Neuromorphic Computing with Memristors: From Devices to Integrated Systems

by

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Abstract

Neuromorphic computing is a concept to use electronic analog circuits to mimic neurobiological architectures present in the nervous system. It is designed by following the operation principles of human or mammal brains and aims to use analog circuits to solve problems that are cumbersome to solve by digital computation. Neuromorphic computing systems can potentially offer orders of magnitude better power efficiency compared to conventional digital systems, and have attracted much interest recently.

In particular, memristors and memristor crossbar arrays have been widely studied for neuromorphic and other in-memory computing applications. Memristors offer co-located memory and logic functions, and intrinsic analog switching behaviors that enable online learning, while memristor crossbars provide high density and large connectivity that can lead to high degree of parallelism. This thesis work explores the device characteristics and internal dynamics of different types of memristor devices, as well as the crossbar array structure and directly integrated hybrid memristor/mixed-signal CMOS circuits for neuromorphic computing applications.

 WO_x -based memristors are used throughout the thesis. Bipolar resistive switching is observed due to oxygen vacancy redistribution within the switching layer upon the application of an applied electric field. In a typical WO_x memristor, oxygen vacancy drift by electric field and spontaneous diffusion result in a gradual resistance change. Depending on the purpose of the applications, the oxidation condition can be varied to achieve either short-term memory or long retention properties, which in turn allow the devices to be used in applications such as reservoir computing or learning and inference. Device fabrication details and device modeling are briefly discussed.

A network structure can be directly mapped onto a memristor crossbar array structure, with one device formed at each crosspoint. When an input vector is fed to the network (typically in the form of voltage pulses), the output vector can be obtained in a single read process, where the inputweight vector-matrix multiplication operation is performed natively in physics through Ohm's law and Kirchhoff's current law. This elegant approach of implementing matrix operations with memristor network can be applied for many machine learning algorithms. Specifically, we demonstrate a sparse coding algorithm implemented in a memristor crossbar-based hardware system, with results applied to natural image processing. We also estimated that the system can achieve $\sim 16 \times$ energy efficiency than conventional CMOS system in video processing.

We further fabricated a 54×108 passive memristor crossbar array directly integrated with all necessary interface circuitry, digital buses and an OpenRISC processor to form a complete hardware system for neuromorphic computing applications. With the fully-integrated, reprogrammable chip, we demonstrated multiple models such as perceptron learning, principal component analysis, and also sparse coding, all in one single chip, with power efficiency of 1.3TOPS/W (estimated at 40nm tech node).

The internal device dynamics, including the short-term memory effect caused by spontaneous oxygen vacancy diffusion, additionally allows us to implement a reservoir computing system to process temporal information. Tasks such as handwritten digit recognition are achieved by converting the spatial information of a digit image into streaming inputs fed into a reservoir composed of memristor devices. The system is also used to experimentally solve a second-order nonlinear task, and can successfully predict the expected output without knowing the form of the original dynamic transfer function.

Other attempts to explore the potential of using memristor networks to solve challenging problems more efficiently are also investigated. Two typical problems, including Hopfield network and self-organizing maps will be discussed.

Chapter 1 Introduction

1.1 Major Roadblocks in Conventional Computing

Nowadays, billions of transistors are working around us in our daily life, powering things from smartphones, personal laptops, automobiles to thermostats and toaster ovens. With the rapid growth of big data processing, Artificial Intelligence (AI) and Internet of Things (IoT), the need of high performance and energy-efficient computing has grown rapidly. However, conventional CMOS—based computing systems are now facing many roadblocks, especially the end of Moore's Law and the drag on system performance due to the von Neumann Bottleneck. With the increasing fabrication cost and impending fundamental physical limits, device scaling becomes ever challenging. On top of it, the energy and speed penalties associated with data movements between the memory and the processor severely limit the systems' performance gains even if device scaling could be continued. The semiconductor industry is forced into exploring solutions based on novel devices and new computing principles. Inspired by biology, neuromorphic computing has become a promising candidate that can provide guiding principles for device innovation and system optimization in the future.

1.1.1 Dying of the Moore's Law

Since Dr. Gordon E. Moore first proposed the famous "Moore's Law" in 1965 and predicted the number of transistors in a dense integrated circuit will double every 18 months¹, it has been guiding the growth of semiconductor industry for many decades. As a result, we as a society have enjoyed the success of ever powerful computing systems which now offer billions of transistors on a tiny chip.

However, Moore's law has started to falter in the last decade and will likely end soon, due to unavoidable heat jammed into small areas that leads to the phenomenon of "dark silicon" where not large portions of devices cannot be utilized, and the upcoming scaling limit when transistor sizes approaches atomic level². To find solutions after the end of Moore's Law, the concept of "Beyond CMOS" was brought up in early 2000s which focuses on device technologies beyond the

CMOS scaling limits³ and "More-than-Moore" which focuses on novel applications with emerging devices and hybrid integrations⁴. Out of the many emerging devices, memristor, or resistive random-access memory (RRAM), has gained broad interest for its ability to address future storage and computing needs. The operations of memristors will be discussed in the next section.

1.1.2 The Von Neumann Bottleneck

Another major roadblock is the so-called "Von Neumann Bottleneck". In 1945, John von Neumann proposed a computing architecture that proscribed separating program and data memory from arithmetic and logical computations⁵. Instructions and operands are to be fetched from memory, a computation performed in the arithmetic-logic unit (ALU), and the results returned to memory.

The von Neumann architecture, however, suffers from a fundamental drawback: the separation of memory and computing elements requires a constant movement of data across a finite width bus (or several busses) in order to perform operations, and this movement requires significant energy and time expenditures.

Recently, with the ever-growing need to handle "big data" and implementing deep neural networks, the von Neumann bottleneck has become a major limitation. Neural networks implemented with the conventional computing hardware will have the synaptic weights stored in (off-chip) memory so that large amount of data need to be transmitted back-and-forth constantly, between the memory and processing units, and requires enormous computing hardware resources and high power consumption during operation.

1.2 Neuromorphic Computing

A more efficient approach towards computing is found in biological systems which must operate on a highly constrained power budget. Take the human brain as an example, arguably the most powerful computer for many tasks. It is estimated from blood flow measurements to be able perform all of its functions while using approximately 20 watts^{6,7}. The brain accomplishes this feat by approximating computational tasks with *analog* physical basis functions to achieve high computational efficiency rather than digital logic basis functions as in traditional computer systems. Additionally, the *learning* and *feedback and adaptation* features allow the system to improve itself from signal statistics and maintain robustness to device and signal errors and to ensure efficient operation in the most informative regions⁷.

Inspired by the human brain, the concept of "neuromorphic computing" was introduced by Carver Mead in early 1990s⁸. It describes a neural information processing paradigm whose physical architecture and design principles are based on those of biological nervous systems. Mead pointed out that the use of the physical basis functions of analog computation, the intimate integration of logic and memory through mostly local wiring, and the learning capabilities of neurobiological systems were key ingredients to their energy efficiency.

To implement a neuromorphic system in computing hardware, we need to find an appropriate electronic device with the capability of performing analog computing, by simultaneously storing the synaptic weight and modulating the transmitted signal to avoid the von Neumann bottleneck. With representation of information by the relative values of analog signals, it can achieve orders of magnitude energy efficiency than conventional digital computation⁹.

Remarkably, memristor can naturally play such a role in neuromorphic computing. Owing to their ability to co-locate memory and compute operations in the same physical device, and their analog switching behaviors caused by ion migration, memristors are ideally suited to realize highly efficient bio-inspired neural networks in hardware.

1.3 Memristors

Memristors, or memristive devices, are two-terminal electrical components whose resistance values depend on the history of applied stimulations. The device states are described by one or a few internal state variable(s) and are typically governed by dynamic ionic processes. Since the device retains its resistance even without power, it is suitable for applications as non-volatile memories. Because it uses its resistance value to represent information, it is a memory resistor, or for short — memristor.

The original concept of memristor was proposed in the 1971 by Prof. Leon Chua at University of California, Berkeley¹⁰. The initial definition of memristor is an electrical element that relates electric charge and magnetic flux linkage, as shown in Figure 1-1. Due to its potential applications in memory and computing systems, memristors have been intensively investigated in the last a few years.



Figure 1-1: Memristor as the forth electrical element along with resistor, inductor and capacitor. Image adapted from Reference [12]. Image credit: Dr. Dmitri B. Strukov.

A typical memristor has a sandwiched metal-insulator-metal (MIM) structure, in which the switching happens in the insulator layer, or so-called switching layer. Due to the simplicity of its structure, memristors can be easily fabricated by inserting the switching material between two crossing metal lines, forming the cell at the crosspoint, as illustrated in Figure 1-2a. This is the so-called "crossbar" structure¹¹, where an array of memristors can be obtained by an array of such devices (Figure 1-2b), offering the highest possible storage density in 2D structures. Such crossbars can also be stacked over each other, further improving the memory storage density.



Figure 1-2: Crossbar structure for memristor. The cell is formed at the cross-point of two metal lines by inserting the switching material. Showing (a) a single cell and (b) a crossbar array. Image adapted from Reference [11]. Image credit Dr. S.H. Jo

The state of a memristor, which provides the memory effect, depends on one or more internal state variables and can be modulated by the history of external stimulation^{10,12–14}. Generally speaking, a memristor's resistance is determined by the internal ion (either cation or anion) configuration, where the re-distribution of oxygen ions or metal cations inside the device modulates the local resistivity and overall device resistance^{12,14–16}.

The key advantages of memristors include the simple structure thus low cost and high memory density, fast speed, low power, and compatibility with conventional complementary metal oxide semiconductor (CMOS) fabrication that allows for hybrid circuit and 3D integration, making them very attractive for a broad range of applications including memory, analog and reconfigurable circuits, as well as neuromorphic computing.

1.3.1 WO_x Memristor Device

The neuromorphic computing systems discussed in this thesis work are based on WO_x memristors. The devices have a metal-insulator-metal (MIM) structure similar to other memristors^{17,18}, and is shown in Figure 1-3. The W bottom electrode (BE) was partially oxidized to form the nonstoichiometric WO_x switching layer. Pd and Au were deposited as the top electrode (TE). The SiO₂ spacer structure was fabricated to enable better step coverage of the top electrodes at the cross points and also restrict the resistive switching regions to a flat surface that is formed at the top of the W BE.



Figure 1-3: Schematic of a WO_x memristor. The device has a MIM structure, with W as the bottom electrode, WOx as the switching layer and Pd as the top electrode.

In a typical device fabrication process, a 60 nm W film is first deposited on a Si/SiO₂ substrate by RF sputtering at room temperature. Then the bottom electrodes are patterned by electron-beam (e-beam) lithography, Ni deposition by evaporation and lift-off, followed by

reactive ion etching (RIE) using Ni as a hard mask to etch uncovered W. After removing Ni by wet etching, rapid thermal annealing (RTA) in pure oxygen at temperatures ranging from 375° C to 450° C, with annealing times ranging from 30 s to 90 s, is performed to partially oxidize the W film and form the nonstoichiometric tungsten oxide layer as the switching layer. The thickness of the WO_x layer ranges from 40 nm to 90 nm depending on the oxidation condition, which in turn leads to different switching behaviors and allows tuning of the device performance for different applications. Finally, the Pd/Au top electrodes, where Au acts as a protective cover layer and also allows better ohmic contact for probe station test and wire-bonding, are patterned by e-beam lithography, evaporation, and lift-off processes. Afterwards, the tungsten oxide regions outside the crosspoints formed between the TEs and the BEs are etched away by RIE, using the TEs as a hard mask. Another photography and metal deposition process, usually NiCr (5 nm) and Au (140 nm), may be performed to form the bonding pads for both the BEs and the TEs to allow wire-bonding of the chip to a chip carrier for measurements using customized testing boards of our group. A scanning electron microscope (SEM) image of a 32×32 memrsitor array is shown in Figure 1-4.



Figure 1-4: SEM image of a fabricated 32×32 WO_x memrsitor array.

1.3.2 Analog Switching



Figure 1-5: DC voltage sweeps on a WO_x memristor, showing gradual state changes. The device conductance was increased during the 3 consecutive positive sweeps (red arrows), then decreased during the 3 subsequent negative sweeps (blue arrows).

As with all memristor devices, a "pinched-hysteresis" behavior can be distinctively observed in the I-V characteristics in the WO_x memristor devices, as shown in Figure 1-5. When a positive voltage is applied, the device conductance gradually increases (termed the write process) and when a negative voltage is applied the conductance gradually decreases (termed the erase process). Moreover, when multiple consecutive positive sweeps are applied, the device conductance continues to increase with each sweep, but also exhibits overlaps between the hysteresis loops, consistent with the short-term memory behavior discussed in refence¹⁷.

The gradual conductance changes can be more clearly observed by pulse measurements, as shown in Figure 1-6. Here 50 write pulses (+1.4 V, 100 μ s) were applied to the device, followed by 50 erase pulses (-1.3 V, 100 μ s). The device state was monitored by a small read pulse (0.5 V, 200 μ s) after each write/erase pulse.



Figure 1-6: Pulse measurements of a WO_x memristor, showing the gradual conductance changes. Positive write pulses (+1.4 V, 100 μs) gradually increase the device conductance (red squares) wile negative erase pulses (-1.3V, 100 μs) gradually decrease the conductance (blue squares).

1.3.3 Device Modeling

The WO_x device characteristics can be explained by the redistribution of ions, here in the form of oxygen vacancies (V_{os}), as has been discussed in previous literatures^{12,19,20}.

Specifically, the memristor dynamics can be described by the following equations:

$$I = (1 - w)\alpha[1 - exp(-\beta V)] + w\gamma \sinh(\delta V)$$
(1-1)

$$\frac{dw}{dt} = \lambda \sinh(\eta V) - \frac{w}{\tau} \tag{1-2}$$

Equation (1-1) is the I-V equation which includes a Schottky (the 1st term) corresponding to conduction in the V_o-poor region and a tunneling-like term (the 2nd term) corresponding to the V_o-rich region. The two conduction channels are in parallel and their relative weight is determined by the internal state variable w.

Equation (1-2) is the dynamics equation which describes the change rate of the state variable w with respect to the applied voltage, including the drift effect under an applied electric field (the 1st term) and the spontaneous diffusion (the 2nd term). $\alpha, \beta, \gamma, \delta, \lambda, \eta$ are all positive-valued parameters determined by material properties. τ is the diffusion time constant, which corresponds to the retention or the decay speed of the memristor device.

During the device fabrication, we can tailor the oxidation conditions to achieve different

device retention performance. With oxidation at a low temperature such as 375° C for 60s, we can achieve the so-called *short-term memory* effect, which refers to the fact that the device can only hold its conductance value for a short period of time (Figure 1-7). This type of memristor can be used in certain applications that takes advantage of the short-term memory dynamics to process temporal information, which will be discussed in Chapter 5. The time constant τ in the short-term memory devices is typically around 50ms.



Figure 1-7: Conductance decay in a WO_x memristor. The device was first programmed by 5 write pulses (1.4 V, 1 ms) then its conductance was monitored by periodic read pulses (0.4 V, 500 μs).

If we use stronger oxidation condition, e.g. 425°C for 60s, the device can obtain much longer retention. In this case, we can use the memristor devices to store synaptic weights and to perform matrix operation directly in the memristor arrays, as introduced in section 1.3.5. Examples of such devices will be mentioned in Chapter 2 to Chapter 4.

1.3.4 Memristor as Synapse

With the ion-driven analog switching behavior, memristors can be used to naturally emulate biological synapses. Synapses are connections between neurons, and provide critical functions to transfer and regulate signals between neurons that form the basis of memory and cognition in biological systems. There are $\sim 10^{11}$ neurons and $\sim 10^{14}$ synapses in a human brain⁷. Neurons and synapses together make up neural networks, which are the building blocks that empower humans

to learn, think and remember.

A key attribute of the brain's computing power is that the synapses are "plastic" – that is, the synaptic weight, or the connection strength between neurons, can be modulated and new weight can be retained. Since the synaptic weight regulates the transmission of signals between neurons, synaptic plasticity along with the very large synaptic connectivity empowers the efficient brain-based parallel computing paradigm and lays the foundation of neuromorphic computing.

The prospect of building biologically inspired neuromorphic computing systems with memristor networks²¹ has generated significant interest since memristors can phenomenologically and bio-realistically emulate synaptic plasticity, and offer the desired large connectivity and low power budget, as illustrated in Figure 1-8²¹



Figure 1-8: Memristors as synapses in a network.

Schematic illustration of the concept of using memristors as synapses between neurons. The insets show the schematics of the two-terminal device geometry and the layered structure of the memristor. Image adapted from Reference [21]. Image credit: Dr. S.H. Jo

1.3.5 Memristor Crossbar Array for Neuromorphic Applications

A network of many memristor devices, formed in the structure of a crossbar array as shown in Figure 1-9, can then be used to implement synaptic weights in general Artificial Neural Network (ANN) applications. In particular, this type of crossbar array structure can perform many tasks that are based on matrix operations efficiently, due to its ability to implement vector-matrix multiplications in a natural and elegant fashion, using Ohm's law and Kirchhoff's current law.



Figure 1-9: Memrsitor crossbar array for neuromorphic computing A memristor is formed at each crosspoint of the crossbar array. In this approach, vector-matrix multiplication can be obtained through Ohm's law and Kirchhoff's law through a simple read operation. Image adapted from Reference [33]. Image credit: Dr. Mohammed A. Zidan

As illustrated in Figure 1-10, if an input vector **x** is fed to the crossbar with each element x_i applied on a row of the crossbar while keeping the columns grounded, the current flowing through each memristor at the crosspoint (*i*, *j*) will be:

$$I_{ij} = x_i w_{ij} \tag{1-3}$$

where x_i represents the vector element which for example could be a pulse with a fixed amplitude and width modulated according to the input, and w_j represents the state of memristor, i.e., the conductance (often called weight in neuromorphic systems). Since all memristors on one column share the same bottom electrode, the current collected at column *j* is the sum of all the currents flowing through the memristors on this column

$$I_j = \sum_{i=1}^n x_i w_{ij} = \mathbf{x} \cdot \mathbf{W}_j \tag{1-4}$$

Therefore, the current measured at column *j* represents the dot product of the input vector **x** and the stored weight vector (often called the feature vector) \mathbf{W}_j in column *j* of the crossbar, $\mathbf{x} \cdot \mathbf{W}_j$. By collecting currents in all the columns, the vector-matrix multiplication (VMM) output, $\mathbf{x} \cdot \mathbf{W}$, can then be obtained in a single "read" operation. This operation best represents the benefits of computing in memristor crossbars – the ability to perform computing in the weight storage devices directly, as well as the high-degree of parallelism where all devices in the crossbar operate in parallel and perform the multiply and add functions simultaneously.



Figure 1-10: Memristor crossbar architecture to calculate vector matrix multiplication. Inputs are applied on the rows as x_i, while the current (charge) is collated on the columns, schematically shown as A_j. Memristors are formed at the crosspoints with the weight w_{ij}.

Moreover, because the resistances of memristors can be readily modulated, neuromorphic systems based on memristors can achieve online learning, by updating the resistances of the memristors that form the feature vectors using voltage pulses with higher amplitudes that can drive the internal ion migrations in the devices.

Due to the compact device structure and the ability to both store and process information at the same physical locations, memristors and memristor crossbar arrays have been extensively studied for neuromorphic computing and machine learning application such as single laye^{22,23} and multi-layer perceptron networks^{24,25}, image transformation^{26,27}, sparse coding²⁸, reservoir computing²⁹ and principal component analysis³⁰. Our approach of implementing neuromorphic applications will be discussed in detail in following chapters.

1.4 Organization of the Dissertation

In this chapter, we have introduced the memristor concept and the crossbar architecture. Our studies are based on WO_x memristor devices, where Figure 1-11 lists the main properties of the device and the appropriate neuromorphic applications it is suitable for.

Specifically, for WO_x devices with long retention, we can store analog information at large scale. Combined with the crossbar configuration, it can be used to perform vector-matrix multiplications. Furthermore, with the gradual analog switching behavior, online learning

algorithms can be implemented in the memristor hardware system. On the other hand, for WO_x devices short-term memory, we can use their internal dynamics for temporal information processing and reservoir computing applications.



Figure 1-11: The WO_x characteristics and the corresponding neuromorphic applications it is suitable for.

The rest of the thesis will discuss a few studies based on the WO_x memristor devices, and is organized as following:

Chapter 2 discusses a sparse coding algorithm that has been implemented experimentally with a WO_x memristor crossbar network. Results of simple bar patterns and complex natural images will be discussed.

Chapter 3 discusses the constraints in online dictionary learning with realistic memristor devices and proposes a solution based on epsilon-greedy strategy to improve training performance.

Chapter 4 discusses a hybrid integrated system with the WO_x arrays directly fabricated on a custom-designed CMOS chip to implement multiple neuromorphic applications on-chip in a functional, standalone system.

Chapter 5 discusses memristor-based reservoir computing, emphasizing the temporal information processing ability of WO_x memristors through its internal dynamics. Examples of digit recognition and temporal signal processing will be presented.

Chapter 6 discusses two other possible neuromorphic applications for further research directions.

Chapter 2 Sparse Coding with Memristor Crossbar Array

From the discussion in Chapter 1, we learned that if constructed into the crossbar structure, memristor networks can efficiently implement matrix operations, especially vector-matrix multiplications (VMM) in parallel and with high energy efficiency. Neuromorphic computing systems can be implemented in hardware based on this approach^{13,31–33}, for tasks such as feature extraction and pattern recognition^{22,23,27,30,34}.

In this study, we experimentally demonstrate a sparse coding algorithm implemented in a memristor crossbar network, and show that the memristor network can be used to perform applications such as natural image processing with an offline learned dictionary set.

2.1 Sparse Coding

Sparse coding aims at representing the original data with the activity of a small set of neurons, and can be traced to models of data representation in the visual cortex^{35,36}. Sparse representation reduces the complexity of the input signals and enables more efficient processing and storage, as well as improved feature extraction and pattern recognition functions^{37,38}.

The concept of sparse coding is as follows: Given an input signal, x, and a dictionary of features, D, sparse coding aims to represent x as a linear combination of features from D using a set of sparse coefficients a, with minimum number of features. Mathematically, the objective of sparse coding can be summarized as minimizing an energy function containing both the reconstruction error term as well as a sparsity penalty term, defined as:

$$\min_{a}(|x - Da^{T}|_{2} + \lambda |a|_{0})$$
(2-1)

where $|\cdot|_2$ and $|\cdot|_0$ are the L^2 - and the L^0 -norm, respectively, and λ is a sparsity parameter that determines the relative weights of the reconstruction error (1st term) and the sparsity penalty (the number of neurons used, 2nd term).

A schematic of the sparse coding concept is shown in Figure 2-1, where an input (e.g. the

image patch of a clock) is represented by a few features selected from a large dictionary^{35,38}.



Figure 2-1: Schematic of the sparse coding concept. An input (e.g., the image patch of a clock) can be decomposed into and represented with a minimal number of dictionary elements. The numbers in the images are just for illustration purpose and are not the actual sparse code.

Sparse representation of information provides a powerful method to perform feature extraction on high-dimensional data, and is of broad interest for applications in signal processing, computer vision, object recognition and neurobiology³⁷. Sparse coding is also believed to be a key mechanism by which biological neural systems can efficiently process complex, large amount of sensory data while consuming very little power^{36,38,39}.

2.2 Locally Competitive Algorithm

The *Locally Competitive Algorithm (LCA)* is a sparse coding algorithm that uses a dictionary of feature vectors (represented by synaptic weights) to transform a vector of input signal into a relatively small number of output coefficients, which can be used for image compression or object recognition⁴⁰.

LCA solves the minimization problem in Equation (2-1) using a network of leaky-integrator neurons and connection weights. Different from commonly used feed-forward neural networks, LCA describes a dynamical system where neurons compete with each other in proportion to the similarity of their respective receptive fields (the collection of synaptic weights entering a neuron). In this approach, the membrane potential of an output neuron is determined by the input, a leakage term, and an inhibition term whose strength is proportional to the similarity of the neurons' features⁴⁰ (an active neuron will try to inhibit neurons with similar features with itself). After the

network get stabilized, an optimal sparse representation, out of many possible representations will be obtained.

Mathematically, in LCA, *x* is an *m*-element column vector, with each element corresponding to an input element (e.g. intensity of a pixel in an image patch). *D* is an $m \times n$ matrix, where each column of *D* represents an *m*-element feature vector (i.e. a dictionary element) and connected to a leaky-integrator output neuron. *a* is a sparse row vector of neuron activity coefficients, where the *i*th element of a represents the activity of the *i*th neuron, whose feature vector is used in the data reconstruction. After feeding input *x* to the network and allowing the network to stabilize through lateral inhibition, a reconstruction of *x* can be obtained as Da^T , and in a sparse representation only a few elements in *a* are nonzero while the other neurons' activities are suppressed to be precisely zero⁴⁰.

The neuron dynamics during LCA analysis can be summarized by Equation (2-2)

$$\frac{du}{dt} = \frac{1}{\tau} \left(-u + x^T D - a(D^T D - I_n) \right)$$
(2-2a)

$$a = \begin{cases} u & \text{if } u > \lambda \\ 0 & \text{otherwise} \end{cases}$$
 (2 - 2b)

where *u* is called neurons' *membrane potentials*, τ is a time constant, and I_n is the $n \times n$ identity matrix.

During LCA analysis, each neuron *i* integrates its input $x^T D$, leakage -u, and inhibition $a(D^T D - I_n)$ terms and updates its membrane potential u_i in Equation (2-2a). If and only if u_i reaches above a threshold (set by parameter λ), neuron *i* will produce an output $a_i = u_i$, otherwise the neuron's activity a_i is kept at 0 (as in Equation (2-2b)).

Specifically, the input to neuron *i* results from the signal *x* scaled by the weights D_{ji} connected to the neuron (second term in Equation (2-2a)). To this regard, the collection of the synaptic weights D_{ji} associated with neuron *i*, corresponding to a feature column of *D*, is also referred to as the receptive field of neuron *i*, analogous to the receptive fields of biological neurons in the visual cortex^{38,41}. A key feature of LCA is that the neurons also receive inhibition from other active neurons (last term in Equation (2-2a)), an important feature in biological neural systems³⁸. LCA incorporates this competitive effect with the inhibition term proportional to the similarity of the neurons' receptive fields⁴⁰ (measured by $D^T D$ in Equation (2-2a)). By doing so, it prevents multiple neurons from representing the same feature and allows the network to dynamically evolve

to find an optimal output. Note that when a neuron becomes active, all other neurons' membrane potentials will be updated through the inhibition term (to different degrees depending how similar the neurons' receptive fields are). As a result, an initially active neuron may become suppressed and a more optimal representation that better matches the input may be found. In the end the network evolves to a steady state where the energy function (Equation (2-1)) is minimized and an optimized sparse representation (out of many possible solutions) of the input data is obtained from a combination of stored features based on the active neurons.

Note however implementing the inhibition effect $D^T D$ can be computationally intensive. On the other hand, the original Equation (2-2a) can be re-written into Equation (2-3) below

$$\frac{du}{dt} = \frac{1}{\tau} (-u + (x - \hat{x})^T D + a)$$
(2-3)

where $\hat{x} = Da^T$ is the signal estimation (i.e. the reconstructed signal). Equation (2-3) shows that the inhibition term between neurons can be reinterpreted as a neuron removing its feature from the input when it becomes active, thus suppressing the activity of other neurons with similar features. By doing so, the matrix-matrix operation D^TD in Equation (2-2a) is reduced to two sequential matrix-vector dot-product operations (one used to calculate $\hat{x} = Da^T$ and the other used to calculate the contribution from the updated input $(x - \hat{x})^TD$), which we show can be efficiently implemented in memristor crossbars in discrete time domain without physical inhibitory synaptic connections between the neurons.

2.3 Mapping Sparse Coding onto Memristor Network

As discussed in Chapter 1, memristor crossbars are particularly suitable for implementing neuromorphic algorithms, because the vector-matrix multiplication operations can be performed through a single read operation in the memristor array^{32,42}.

We experimentally implemented the sparse coding algorithm in the memristor array-based artificial neural network, schematically shown in Figure 2-2. In this implementation, x is an melement column vector applied to the rows of the memristor crossbar (cyan pads on the left), with each element corresponding to an input element (e.g. intensity of a grayscale pixel in an image patch). It is implemented by read pulses with a fixed amplitude but variable width proportional to the pixel intensity.



Figure 2-2: Schematic of memristor crossbar based computing. A memristor is formed at each crosspoint and can be programmed to different conductance states (represented as grayscale color).

In this approach, the dictionary, D, is directly mapped element-wise into the memristor crossbar with each memristor at row i and column j storing the corresponding synaptic weight element D_{ij} . The input vector x (*e.g.* grayscale pixel intensities of the input image when used in image analysis) is implemented with read pulses with a fixed amplitude and variable width proportional to the pixel intensity. As a result, the total charge Q_{ij} passed by a memristor at crosspoint (i,j) is linearly proportional to the product of the pixel intensity x_i and the conductance D_{ij} of the memristor $Q_{ij} = x_i D_{ij}$, and the charge passed by all memristors sharing column j is summed via Ohm's Law and Kirchhoff's current law: $Q_j = \sum_i x_i D_{ij} = x^T D_j$ (Figure 2-2). In other words, the total charge accumulated at neuron j is proportional to the dot-product of the input xwith the neuron's receptive field D_j .

Since the dot-product of vectors measures how close the input vector is matched with the stored vector, the ability to implement this operation in a single read process allows the memristor network to conveniently and efficiently perform this important pattern matching task. This term $(x^T D \text{ in vector form})$ is then added to the neuron's membrane potential following Equation (2-3), a leakage term is subtracted, and the membrane potential is then compared to the threshold parameter, λ . If the membrane potential is above threshold λ , the neuron is active for the next phase.

In the second phase, the input image is reconstructed using the currently active neurons and compared to the original input. This is accomplished by performing a "backward read": variable

width read pulses, proportional to the neurons' activities a_j , are applied on the columns while the charge is collected on each row *i* to obtain $Q_i = \sum_j D_{ij} a_j = D_i a^T$. This backward read has the effect of performing a weighted sum of the receptive fields of the active neurons, and the total integrated charge on the rows is proportional to the intermediate reconstructed signal $\hat{x} = Da^T$ in vector form. The difference of *x* and \hat{x} , referred to as the residual, is used as the new input to the array to obtain an updated membrane potential. The forward and backward processes are repeated, alternately updating the neuron activities and then the residual. The updated value is calculated from Equation (2-2) and (2-3) by a FPGA board in the measurement setup. After the network has stabilized, a sparse representation of the input, represented by the final output activity vector *a*, is obtained. By performing these forward and backward passes in the same memristor network in discrete time domain, we can effectively achieve lateral inhibition required by the sparse coding algorithm, without having to implement physical inhibitory synaptic connections between neurons.



Figure 2-3: Memristor crossbar network for sparse coding. Upper right inset shows a magnified scanning electron microscope (SEM) image of the crossbar. Lower left inset shows the memristor chip integrated on the testing board after wire-bonding.

In this study, the hardware system used is a 32×32 memristor crossbar array, where a memristor formed at each intersection in the crossbar (Figure 2-3). The WO_x memristor devices are fabricated by Dr. Chao Du following the previously developed proocess¹⁸ discussed in Chapter 1. When fabrication is completed, the memristor crossbar array chip is wire-bonded and integrated on a custom-designed testing printed circuit board (PCB), as shown in the lower inset of Figure 2-3. Dr. Patrick M. Sheridan and Zelin Zhang also helped tremendously in building the hardware and

software of testing platform.

During experimental measurements, the original input (for example an image) is fed to the rows (which are the top electrodes) of the memristor array and the columns (which are the bottom electrodes) of the array are connected to output neurons. The memristor network performs critical pattern matching and neuron inhibition operations to obtain a sparse, optimal representation of the input. After the stabilization of the memristor network, the re-constructed image can be obtained based on the (sparse) output neuron activities and the features stored in the crossbar array.

2.4 Sparse Coding Results of Simple Inputs

To experimentally demonstrate sparse coding with the memristor network, we start with simple inputs such as grayscale horizontal and diagonal bar patterns for image reconstruction.

The first demonstration is encoding an image composed of diagonally oriented stripe features using the algorithm given above. The dictionary, shown in Figure 2-4a, contains 20 features with each feature consisting of 25 weights. The 20 features were written into the 20 columns (with each weight represented as a memristor conductance) and the inputs were fed into the 25 rows, which means a 25×20 sub-array was used out the 32×32 memristor array in this experiment. An input signal, shown in Figure 2-4b and consisting of a combination of 4 features, is used as a test input to the system.

The network stabilizes after 30 forward-backward iterations, and the final signal reconstruction is shown in Figure 2-4b. It can be seen that the input image can be correctly reconstructed with neurons 2, 6, 9, and 17, corresponding to the features of the input, weighted by their activities. Additionally, the experimental setup allows us to study the network dynamics during the analysis.



Figure 2-4: Experimental demonstration of sparse coding using memristor network. a) Dictionary elements programmed into the memristor crossbar array, each dictionary element is stored in a single column. b) The original and the reconstructed image after the memristor network settles. c) Membrane potentials of the neurons as a function of iteration number during LCA analysis. Red horizontal line: threshold parameter. d) Additional examples of input images and reconstructed images.

Figure 2-4c plots the membrane potential values for all 20 neurons during the iterations. It can be seen that for the first 2 iterations, all neurons are charging (at somewhat different rates depending on how well the input is matched with the stored receptive fields, which is in turn affected by device variabilities) and none are above threshold. After the 4_{th} iteration, the membrane potentials of 11 neurons (numbers 1, 2, 4, 5, 6, 9, 10, 13, 14, 16, 17) have exceeded the threshold. Out of these 11 neurons, the receptive fields of neurons 2, 6, 9, and 17 match the features in the input, while those of neurons 1, 4, 5, 10, 13, 14, 16 are not perfect matches but still overlap enough with the input image to allow these neurons to be charged at reasonable rates. In the subsequent backward read, all the active neurons will contribute their receptive fields to the reconstruction, and result in a reduced residual input. As a result, there is a reduction in the charging rates and a decrease of the neurons' membrane potentials at iteration 5 due to the leaky term in Equation (2-3). Over the next a few iterations the lateral inhibition between neurons eventually drives the membrane potentials of neurons 1, 4, 5, 10, 13, 14, 16 below the threshold in the 10th iteration and keep these neurons inactive in subsequent iterations. The inactive neurons' membrane potentials

continue to decay due to the leakage term, but because they are below threshold, their values have no impact on the final sparse code. In the end, a correct and sparse representation of the input is reconstructed in Figure 2-4b based on the active neurons 2, 6, 9, and 17 after the network stabilizes.

This experiment demonstrates an important feature of the sparse coding algorithm: lateral inhibition mechanisms drive the system to accurately represent the input. Non-idealities in the memristor network may temporarily lead to incorrect behavior (as in the case of the 4th iteration or the 8th iteration when neurons 4, 14, 16 exceed the threshold), but the lateral inhibition inherent in the neuron dynamics can effectively correct these errors. These features of the network dynamics have been further analyzed through simulations of the memristor crossbar-based sparse coding hardware. Additional examples of inputs composed of two features and the reconstructed images from the memristor crossbar can be found in Figure 2-4d.



Figure 2-5: Sparse coding using more overcomplete dictionary.
 a) Dictionary elements based on horizontal and vertical bars programmed into the memristor crossbar array.
 b) The original image to be encoded and the reconstructed image after the memristor network settles.
 c) Membrane potentials of the neurons as a function of iteration number during LCA analysis. Red horizontal line: threshold parameter.

The re-programmability of memristors allows the dictionary set to be readily adapted to the types of signals to be encoded, so the same memristor hardware system can process different types of inputs using a single general approach. To demonstrate this point, we re-programmed a new dictionary composed of horizontally and vertically oriented bars (Figure 2-5a) into the same array used in studies in Figure 2-4. By using this new dictionary, images consisting of bar patterns can be efficiently reconstructed using the same algorithm. More importantly, in order to demonstrate the capability of sparse coding to find the optimal solution out of several possible solutions, a dictionary that is larger than the input space, e.g. a so-called over-complete dictionary set⁴⁰, is used
in the examples shown in Figure 2-5a, the dictionary is minimally over-complete (since the input is restricted to be the combinations of the diagonal stripe features and corresponds to an input dimensionality of 17, determined from the linear span of the features). By using the bar patterns in Figure 2-5a and restricting the input images to only combinations of horizontal and vertical bars, the input dimensionality is reduced to 9. With a total of 20 stored dictionary elements, the system now achieves greater than $2\times$ over-completeness in such a relatively small network and should be better to highlight the effects of sparse coding.

The resulting reconstructions using this overcomplete dictionary are shown in Figure 2-5b and Figure 2-5c. The network not only correctly reconstructed the input image, but as expected, it picked the more efficient solution – a solution based on neurons 8 and 16, over another solution based on neurons 1, 4, and 8. As can be seen from Figure 2-5c in the first 5 iterations, all neurons are charging and the membrane potentials of neurons 1, 4, 8 and 16 first cross the threshold at iteration 6. Even though the receptive fields of all the four neurons (1, 4, 8 and 16) are correct features in the input, neurons 8 and 16 (consisting of two bars) represent a sparser representation. As a result, inhibition implemented in the system eventually suppresses the membrane potentials of neurons 1 and 4 to be below the threshold after iteration 11 and keeps them below the threshold after the network stabilizes. As a result, the activities of these two neurons are set to be precisely 0 (Equation (2-2b)), and an optimal solution based only on neurons 8 and 16 is obtained, compared to other possible, less-sparse solutions.



Figure 2-6: Additional examples of input images and reconstructed images. The same threshold $\lambda = 40$ is used in all experiments.

To further demonstrate the performance of the robustness of the hardware system, an exhaustive test of all 50 patterns consisting of two horizontal bars and one vertical bar were performed (Figure 2-6) with a success rate of 94% (measured by the network's ability to correctly identify the sparse solutions), despite variabilities inherent in the memristor devices.

2.5 Sparse Coding Results of Natural Images

Other than simple inputs like bar patterns, we have also demonstrated that our memristor network can perform sparse coding for more complex and interesting input patterns, such as grayscale natural images, using the sparse coding algorithm and a learned dictionary.

In this study, a 16×32 subarray was used out of the 32×32 memristor array, corresponding to a $2\times$ overcomplete dictionary with 16 inputs and 32 output neurons and dictionary elements. The dictionary elements were learned offline using 4×4 patches randomly sampled from a training set consisting of nine natural images (with sizes of 128×128 pixels), using a realistic memristor model and an algorithm based on the winner-take-all (WTA) approach and Oja's learning rule⁴³. More details on the training process can be found in Chapter 3.

After training, the obtained dictionary elements were programmed into the physical 16×32 crossbar array (more details will be discussed in Section 2.6). Using the trained dictionary, we successfully performed reconstruction of 120×120 pixel grayscale images experimentally using the 16×32 memristor crossbar. During the process, the 120×120 input image (Figure 2-7a) was divided into 4×4 patches and each patch was experimentally processed using the memristor crossbar and the Locally Competitive Algorithm (Figure 2-7b). After the memristor network stabilized (typically after 80 forward/backward iterations (Figure 2-7d), the patch was reconstructed using the neuron activities and the corresponding receptive fields stored in the crossbar array, as shown in Figure 2-7c.



Figure 2-7: Natural image reconstruction using memristor crossbar.
a) Original 120×120 image, which is divided into 4x4 patches. b) A 4×4 patch from the original image. c)
The experimentally reconstructed patch with memrsitor network. d) Membrane potentials of the neurons as a function of iteration number during LCA analysis. Red horizontal line: threshold parameter.

The complete image was then composed from the individual patches, shown in Figure 2-8. The reconstructed successfully captured the main features of the original Lena image.



Figure 2-8: Experimental LCA image reconstruction 120×120 Lena Image

To further demonstrate the functionality of the hardware sparse coding system, we tested five other commonly studied images, with different color tones (e.g. with a black or white background) and different features, shown in Figure 2-9. As can be seen from the results, the memristor-based sparse coding system can perform satisfactory reconstruction for all cases, regardless of the content of the figures.



Figure 2-9: More experimental LCA reconstruction results with 120×120 images.

2.6 Nonideality Effect on Image Reconstruction with Sparse Coding

We note the reconstructed images in Figure 2-8 and Figure 2-9 were still not perfect, both experimentally and in the simulation. The imperfect image reconstruction can be caused by serval reasons:

First, due to the device to device variations, the dictionary programmed into the memristor array is not exactly the same as the ideal dictionary obtained from training, and only maintains the major features of the original dictionary elements.

Moreover, due to the limited dictionary size, the small basis space limits the types of features in the trained dictionary to be mainly low-spatial frequency features. The system thus cannot reconstruct the high-spatial frequency features effectively, which leads to lack of fine-grained details in the final image.

Another reason lies in the limitation of the learning algorithm itself, which will be discussed in detail in Chapter 3. In this section, we will focus on the first two issues.

2.6.1 Effect of Device-to-Device Variations

During the natural image reconstruction with offline learned dictionary, the obtained dictionary elements need to be programmed into the physical 16×32 crossbar array. However, since the memristor crossbar array has intrinsic device-to-device variations, the stored dictionary will not be exactly the same as the ideal leaned dictionary. The effect of the device variations on the experimentally stored dictionary is shown in Figure 2-10.



Figure 2-10: The trained dictionary before (a) and after (b) programmed into the crossbar array With the intrinsic device variations, the dictionary after programmed is slightly distorted from the ideal version.

Figure 2-10b shows the dictionary elements experimentally stored in and read out from the memristor crossbar and used for the experimental natural image reconstructions. Due to intrinsic device variations, the patterns stored in the array (Figure 2-10b) are slightly distorted from ideal dictionary (Figure 2-10a), but generally maintain the main features of the learned dictionary elements. Here the dictionary set was written into the array using a single shot method, without repeated read verification and re-programming steps.

This nonideal stored dictionary is one of the reasons of the imperfect image reconstruction. To verify the validity of our experimental approach, we performed a realistic simulation using a device model that incorporates device variations during the weight changes, so that we can repeat effect of the nonideal device variation on the image reconstruction.

To model the device variations during weight updates, we experimentally measured the incremental conductance changes in 288 devices in the memristor array using pulsed programming/erasing conditions. The results are shown in Figure 2-11. Here each device was programmed with 20 write pulses and followed by 20 erase pulses, and the device conductance was monitored after each write/erase pulse by a read pulse.

We fitted the experimental data with the memristor model we discussed in Chapter 1

$$I = w(\gamma \sinh(\delta V)) + (1 - w) \left(\alpha \left(1 - e^{-\beta V} \right) \right)$$
 (2 - 4a)

$$\frac{dw}{dt} = \eta_1 \sinh(\eta_2 V) F(w, V) \qquad (2-4b)$$

where Equation (2-4a) is the current-voltage equation dependent on the internal state variable w, and Equation (2-4b) describes the update rate of the state variable. Since we the device in the sparse coding applications have long retention performance, we can ignore the τ term in Equation (2-4b).

F(w, V) is a window function, which is used to fit the asymmetricity in write and erase:

$$F(w, V) = \begin{cases} 1 - w, & \text{if } V > 0\\ w, & \text{if } V < 0 \end{cases}$$
(2-5)

In our device model we assumed that the initial values of the state variable (w₀) from different devices follow the same Gaussian distribution as observed in Figure 2-11b. During weight updates, we further assumed that the parameters η_1 and η_2 in the weight update equation (Equation (2-4b)) are different for different devices, also following Gaussian distributions. With these modifications to the original ideal device model, the experimentally observed variations during weight updates can be realistically accounted for, as shown in Figure 2-11c, for the same programming/erasing conditions used in the experiments. Exact parameters used in the model are shown in Table 2-1.



Figure 2-11: Experimental pulse write and erase curves from 288 memristor devices (a) Pulse write/erase data measured from 288 devices in the memristor array. (b) Initial conductance distributions. (c) Simulation fitted 288 memristor devices using device model with device-to-device variations (d) Simulation fitted initial conductance distribution

$p(w_o = w) = \frac{1}{\sqrt{2\sigma^2 \pi}} e^{-\frac{(w-\mu)^2}{2\sigma^2}}$				
μ	0.03	α	10 ⁻⁸	
σ	0.009	β	0.5	
γ	10-5	η_1	9×10^{-8} with 3% variation	
δ	4	η_2	15.5 with 1% variation	

Table 2-1: Experimentally extracted parameters used in the device model simulation.

Non-idealities during the dictionary storage were simulated based on the weight update equation from our device model, after considering device variation effects. It can be observed in

Figure 2-12 that our device model can successfully captured the device-to-device variation effect on the dictionary programming.



Figure 2-12: Verification of the device variation on dictionary programming (A) Experimentally stored dictionary elements in the memristor crossbar. (B) Simulated stored weights after considering device variations.

Furthermore, in Figure 2-13, simulations of image reconstruction were then performed using the simulated stored dictionary elements, following the same procedure as the experimental processes. The simulation results consistently reproduced the experimental results (Figure 2-13b) for this image processing task.



Figure 2-13: Verification of the device variation effect on image reconstruction a) Experimentally reconstructed image based on the reconstructed patches. b) Simulated reconstructed image using offline trained dictionary based on WTA.

2.6.2 Effect of Limited Dictionary Size

Another limitation of the current experimental sparse coding setup is the limited dictionary size. Although the dictionary is $2\times$ over-complete, there are still only 32 features in total in the dictionary. As a result, the performance of the reconstruction of natural images, which are generally complex and include both low- and high-spatial frequency features, will not be perfect with these small dictionaries limited by the current experimental setup.

Despite the limits of the small dictionary size, during the process of each 4×4 patch the system was still able to perform reconstruction following the LCA algorithm based on the features in the dictionary, as shown in Figure 2-7. To have a closer look at the details of the image reconstruction results, we show below several additional zoomed-in areas of the original Lena image (Figure 2-14) compared with experimental and simulation reconstruction results (Figure 2-15).



Figure 2-14: Selected regions in the Lena image used for comparison.

As can be seen from Figure 2-15, the experimental reconstruction based on the memristor array can clearly capture key features of the original image, albeit with a lower resolution due to the lack of high-spatial frequency features in the dictionary as discussed earlier. For instance, we can clearly observe the shape of the eyeballs in example Figure 2-15(a), where distinct differences between patch to patch can be seen. Other examples Figure 2-15(b-e) also demonstrate the experimental system's ability to capture continuous edges and shades within and across multiple patches, without overlapping the patches during reconstruction.



Figure 2-15: Comparison of the highlighted regions showing the original, experimental and simulated reconstruction results.





Reconstructed with 96 Elements

Reconstructed with 128 Elements



Reconstructed with 64 Elements



Reconstructed with 160 Elements

(b)

(a)



Figure 2-16: Effect of improvement by using larger dictionary

(a) Simulated reconstructed images with different dictionary sizes. (b) Results from the zoomed-in eye region (marked in the original image in (a)), showing fine features can be captured with increased dictionary size.

To further verify that the apparent limited resolution of the reconstruction is due to the limited dictionary size in this prototype system, we performed extended simulation studies to analyze the effect of the dictionary size on the reconstruction results. As can be seen in Figure 2-16, with the increase of the dictionary size, from 32 features to 64, 96, 128 and 160 features while keeping the input size and all other parameters fixed, the quality of the reconstruction improves. This effect is also more clearly illustrated by showing results in the marked region (Figure 2-16b). The fine features can now be captured by simply increasing the dictionary size

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while keeping all parameters fixed. These analyses verify the potential of using memristor networks to perform image analysis tasks, if the network size can be increased to a more practical size (*e.g.* from 16×32 used in the prototype system to larger sizes such as 16×160 in the future).

2.7 Benchmarking of Sparse Coding for Video Processing

Many real-world applications such as video processing are well suited for sparse coding. We carried out analysis on how the memristor-based hardware will perform in video processing tasks. Figure 2-17 shows an example of a 256×192 grayscale image, which was down-sampled from an original 640×480 image. The image was then processed by the 16×32 memristor crossbar using 4×4 patches. During the process, 3072 (64×48) 4×4 patches were processed using the LCA algorithm and each patch took 300 iterations to allow the network to stabilize. Due to the limited data transfer rate between the memristor array and the digital circuitry in the existing test board, the current memristor board will not be able to perform this video analysis in real time. However, in an integrated memristor/CMOS system with a minimum possible read pulse width of 10 ns, our analysis shows that it will take 0.034 second to process such an image, meeting the requirement of real-time streaming video analysis at a rate of 24 frames/s (<0.042 second process time per frame).





Figure 2-17: 256×192 video frame reconstructed using 4×4 patches using the 16×32 memristor crossbar. To process standard 480p (640×480) videos with at least 24 frames/second frame rate without down-sampling, larger patches (*e.g.* 10×10) will be needed. A memristor array size of 100×200 will be able to process the 480p videos in real time using 10×10 patches. Figure 2-18 shows simulation results of image reconstruction using the larger memristor array.



Figure 2-18: 640×480 video frame reconstructed using 10×10 patches with a 100×200 memristor crossbar.

We then compared the performance of the memristor system with efficient digital solutions. For a fair comparison of the crossbar-based analog solution with a digital solution, both methods need to be subjected to the same constraints, as tradeoffs can always be made between low energy consumption, fast speed and high reconstruction accuracy. In this application, we are targeting power and processing time as the main performance metrics for both systems.

To achieve the benchmarking results, we designed and analyzed an efficient digital system using efficient multiply-accumulation (MAC) circuits. Since an $a \times b$ crossbar can perform the $(1 \times a)$ \times (a×b) vector-matrix dot-product operation in *one* read process in the memristor system, the digital CMOS system was designed to match the same performance. Specifically, for benchmarking purpose we assumed that in an integrated memristor chip a read speed of 10 ns can be achieved. To obtain similar performance in the digital system, we used 4-bit \times 4-bit multiplications to approximately match the dynamic range of the input and the stored values in the memristor crossbar. In the analysis, we used 10×10 patches (aimed for real time processing of 480p video) to sample and reconstruct the image. A 100×200 memristor crossbar was assumed for the memristor implementation. The equivalent digital system in 40 nm CMOS uses 1600 MAC circuits (8 MAC circuits per column and 200 columns operated in parallel) to accomplish one $(1 \times 100) \times (100 \times 200)$ vector-matrix dot-product operation in 10.4 ns. Schematic and parameters of the digital system are shown in Figure 2-19 and Table 2-2: Equivalent digital CMOS design of a 100×200 crossbar using 40nm CMOS Technology, respectively. This design occupies 0.306 mm² and it is estimated to consume 274 mW during the forward pass (reconstruction phase) stage and 548mW during the backward pass (residual calculation) stage.



Figure 2-19: Architecture of the digital CMOS system

with 1,600 4b×4b multipliers, 8 per column; 1,600 adders, 8 per column; and 8 multiplication and accumulation (MAC) per clock cycle per column. Each MAC operation is pipelined to 3 stages. Latency: 16 clock cycles to complete one (1×100) × (100×200) vector-matrix dot-product operation.

	(1×100) × (100×200) operation
Number of Multiply-accumulate (MAC)	1600
Number of pipeline stages	3
Clock period (ns)	0.65
Latency (ns)	10.4
Power consumption (mW)	274
Silicon area (mm ²)	0.306
Power efficiency (TOPS/W)	7.02
Area efficiency (TOPS/mm ²)	6.28

Table 2-2: Equivalent digital CMOS design of a 100×200 crossbar using 40nm CMOS Technology

The comparison between the memristor solution and the digital solution is shown below in Figure 2-20 and Table 2-3: Performance comparison between the memristor solution and the digital solution. The test is based on reconstructing 640×480 natural images at a rate of >24 images/second (*e.g.* real time processing of 480p videos).



Original Image

Memristor solution

Digital solution

Figure 2-20: Image reconstruction results based on a memristor system and an efficient digital approach.

	MSE	L_0	Time	energy
Memristor	1.933×10 ⁻³	15.6%	0.03607s	719.0µJ
Digital	2.226×10 ⁻³	11.3%	0.02636s	11.82mJ

Table 2-3: Performance comparison between the memristor solution and the digital solution

As can be observed from the simulation results, the speed, error and sparsity parameters are similar for the digital solution and the memristor solution, by design. The digital solution resulted higher mean square error but lower L_0 . These can be explained by the quantization effect of the digital approach. In the digital implementation, the synaptic weights were quantized into 4 bits (16 levels), which leads to a quantization error and subsequently slightly higher reconstruction error.

When it comes to power consumption, on the other hand, the memristor analog solution, based on parameters used in the current prototype devices, already demonstrates significant (~16×) improvement over the already very efficient digital solution. This is due to the fact that the vector-matrix multiplication is obtained in a single step by a parallel read process in the memristor system. To achieve the similar throughput in the digital system, eight 4b×4b multipliers were needed in a single column, leading to higher energy consumption. We expect the advantage of the memristor system will be even more pronounced for more complex tasks and with further optimized devices, since in the digital solution analysis we neglected the time and energy costs associated with moving data between the memory (not considered in this simple analysis) and the MAC circuitry, which will not be negligible for larger input data, while in the memristor system such data movement is not needed since the computation is directly performed in the same physical locations as the stored weights. The energy cost in the memristor system can also be significantly lowered further by

optimizing the memristor devices, *i.e.* by using lower current memristor devices.

2.8 Conclusion

Utilizing the merits of memristor crossbar network, i.e., natural implementation of vectormatrix multiplication and weight storage/modulation, an important neuromorphic algorithm, LCA, is demonstrated experimentally on a fabricated WO_x memristor crossbar array. The algorithm can be used to code and reconstruct patterns and images under desired sparsity constraints.

Beyond encoding bar patterns, we demonstrated that the memristor array can be used to experimentally code and reconstruct natural images. The dictionary elements were obtained offline using a realistic memristor model and an approach based on winner-take-all (WTA) and Oja's learning rule. The obtained dictionary elements were programmed into a physical 16×32 crossbar array. Using the trained dictionary, we successfully preformed reconstruction of 120×120 pixel grayscale images using the 16×32 memristor crossbar array.

Furthermore, with a benchmark of video processing simulation, we have demonstrated that with comparable image processing throughput, the memristor sparse coding system can achieve around $16\times$ energy efficiency than a classic CMOS digital implementation using the current devices, with higher efficiency expected with future device and architecture optimizations.

Chapter 3 Online Dictionary Learning with Nonideal Memristor Network

The Locally Competitive Algorithm (LCA), as described in Chapter 2, is mainly focused on inference, which is to represent an input with a given dictionary. The dictionary used in LCA implementation is learned offline in software. However, since the conductance state of memristor devices can be dynamically fine-tuned, memristor crossbar arrays have the potential to perform online learning in hardware, including feature vector learning for feedforward networks (which will be further discussed in Chapter 4) as well as dictionary learning for sparse coding.

A conventional approach for online dictionary learning is to learn through sparse coding, with the learning rule of stochastic gradient descent (SDG). It usually requires some image preprocessing, say whitening and mean removal, to improve training efficiency, which increases the complexity of hardware implementation. Even without image preprocessing, dictionary learning through sparse coding can be time consuming and computationally expensive and is not a very hardware-friendly approach taking into consideration the model complexity and device limitations. These limitations lead us to explore a more suitable algorithm.

Instead, in our experimental LCA implementation we proposed an alternative learning algorithm based on Oja's learning rule in conjunction with winner-take-all (WTA), which enabled fast training of the network to achieve excellent reconstruction performance⁴³. However, when considering experimental constraint of relatively large learning rate and lack of normalization, the dictionary elements can be unevenly trained, leading to badly-learned dictionary.

In this section, we discuss our approach to learn the dictionary of feature primitives using memristor crossbar array, in the presence of device nonideality and realistic experimental constraints. Specifically, an epsilon-greedy strategy is applied to winner-take-all algorithm to avoid uneven training through dictionary elements due to large device to device variations.

Ideally, one would also like to perform online learning experimentally using the same memristor crossbar system. However, the slow speed of the board combined with the large training set prevented us from experimentally implementing online learning in the memristor crossbar. To test the feasibility of online learning we instead performed a detailed, realistic simulation using a device model that incorporates device variations during the incremental weight updates (see Section 2.6.1).

3.1 Dictionary Learning through Sparse Coding

Online dictionary learning can be achieved by using sparse coding algorithm combined with gradient descent, in which sufficient number of training patches are fed into the network and sparse coefficients are obtained by using the sparse coding algorithm, followed by weight updates to reduce the reconstruction error. Stochastic gradient descent is often used instead of batch gradient descent to speed up the learning approach due to the large number of training samples used in the process.

In our SDG implementation, we first initialized the memristor dictionary to random values, and then for each training sample, we obtained the residual error $(x - D^T a)$ following the sparse coding algorithm (which in our case is LCA), and updated the memristor weights directly by increasing or decreasing their values according to the stochastic gradient descent rule, which is described as:

$$\Delta \Phi^{\mathrm{T}} = \beta (x - D^{\mathrm{T}} a) \otimes a \tag{3-1}$$

where *D* is the matrix of dictionary elements (receptive fields), \otimes is the outer product, $x - D^T a$ represents the reconstruction error with $D^T a$ being the reconstructed input based on LCA, and β is the learning rate factor. Note that the dimension of $(x - D^T a) \otimes a$ is the same as the weight matrix.

This learning approach usually includes a mechanism to control and rescale the ℓ_2 -norm of the dictionary elements. Without such a mechanism, the norm of *D* would arbitrarily go to infinity, leading to small values for the coefficients a_i^{44} .

In Chapter 2, the dictionary is trained offline in software and then programmed into the physical array. To train the network, 4×4 patches are randomly sampled from a training set of nine natural images (128×128 pixels) as the training input, shown in Figure 3-1.



Figure 3-1: Training set used to obtain the dictionary

3.1.1 Dictionary Learning with Whitening

Some preprocessing methods are usually taken before online dictionary learning, such as whitening and mean removal, to improve the learning efficiency in many algorithms. As discussed in Olshausen & Field³⁵, high spatial features in the dictionary may be more effectively trained using a whitening technique that filters out the low spatial frequency components. Specifically, a combined whitening/low-pass filter with a frequency response shown in Equation (3-2) has been shown to lead to desired performance:

$$R(f) = f e^{-\left(\frac{f}{f_0}\right)^n}$$
(3-2)

The same combined whitening/low-pass filter was used to pre-process the image patches before training, where f_0 was chosen to be 200 cycles/picture and *n* was set to be 4.

The training data were sampled from ten 512×512 natural images with 12×12 patches. Before the training, all patches were pre-processed using the combined whitening/low-pass filter shown in Equation (3-2). Figure 3-2 shows the original image before and after whitening, as well as the profile of the combined whitening/low-pass filter in frequency domain.



Figure 3-2: The original image before and after whitening along with the profile of the whitening/low-pass filter plotted in frequency domain. 12×12 whitened image patches, randomly sampled from the image set, were used as input

patches for dictionary training, following previous mentioned gradient descent training algorithm.

Figure 3-3 shows the 576 dictionary elements after training (using 12×12 image patches and a $4 \times$ overcomplete dictionary). Similar to results obtained in Zylberberg *et al.*, which used a comparable sparse-coding algorithm³⁹, small unoriented features, oriented Gabor-like wavelets, and elongated edge-detectors can be learned in the dictionary.



Figure 3-3: Receptive fields obtained from gradient descent training using pre-preprocessed images. The resulting fields were sorted using the ratio of the variance over the mean. The gray tone represents zero in all fields, with lighter/darker pixels corresponding to positive/negative values.

An example of image reconstruction using the whitened images and the trained dictionary in Figure 3-3 is shown in Figure 3-4, demonstrating high quality reconstruction using dictionary learned with whitened inputs.



Figure 3-4: Reconstructed image with LCA and online learned dictionary **a** Original whitened image. **b** Reconstructed image using the dictionary in Figure 3-3

It worth mentioning that in this simulation, neither the device model nor the non-ideality is used. The simulation is just aimed to verify the quality of the algorithm. We will discuss the effect of device model in the following section 3.1.2.

3.1.2 Dictionary Learning with SGD and Device Variations

Although the classic sparse coding approach can lead to excellent reconstruction results as shown in Figure 3-4, the whitening preprocessing can lead to a reduced input dynamic range and create negative input values, which increase the complexity of hardware implementation.

Therefore, we consider a simpler approach without the preprocessing of whitening. We directly mapped the original grayscale image value to pulsewidth and performed the online learning with SGD, without mean removal. We use 8×8 patches in this study instead of previously used 4×4 patches, since larger patches can capture higher spatial frequency features more easily during the stochastic gradient descent approach⁴⁵. The dictionary after learning is shown in Figure 3-5.



Figure 3-5: The 8×8 dictionary learned from stochastic gradient descent training. The device variations with experimentally extracted parameters are incorporated in the online learning process.

During the simulation of training, we also included realistic memristor device nonidealities such as device variations, as has been discussed in section 2.6.1, to observe the effect of device model and variations on the result of online learning. Further simulation of the sparse coding with online learned dictionary with this approach shows that high quality image reconstruction can still be obtained even in the presence of realistic device variations (Figure 3-6) if the dictionary is learned online using the memristor crossbar (which was not implemented experimentally in this study due to the limited throughput of the present testing system), where device variations were carefully considered both in terms of conductance variations and weight update rate variations during the learning stage.

This effect can be explained from the fact that the learning algorithm is self-adaptive and adjusts to the device variabilities during the training stage. As a result, online learning can more effectively handle device variations and is particularly suitable for emerging devices such as memristor-based systems where large device variations are expected.



Figure 3-6: Sparse coding with stochastic gradient descent (SGD) a) Reconstruction obtained using ideal dictionary learned via sparse coding and gradient descent. b) Reconstruction obtained using dictionary learned using the memristor device model by considering realistic device variabilities during online learning. 8×8 patches were used during training and image reconstructions in a-b

3.2 Learning with Winner-take-all and Oja's Rule

Although online dictionary learning with stochastic gradient descent and sparse coding can achieve excellent performance, the approach has several major issues when being implemented in hardware:

- 1. The training requires a significant amount of time and resources. For each training sample, the LCA algorithm must run until steady state to obtain the representation coefficients, and then training pulses must be applied for each active neuron. A typical training may take thousands of training samples, which takes significant resources and time to train effectively.
- 2. The learning process requires normalization of the weight vectors, and also leads to negative as well as positive weights. Normalization is a non-trivial process since it requires complex mathematic calculation and modification of all conductances in each column. Moreover, negative weights require differential implementation or other mapping functions involving multiple devices or steps.

Considering these issues with the conventional online learning approach, we proposed an alternative learning algorithm based on Oja's rule with a winner-take-all (WTA) strategy⁴³ for easy

implementation in the hardware for image processing and other tasks.

Oja's rule is a modification of Hebbian learning rule and converges to the principal component with unit Euclidian norm⁴⁶. In our approach, the WTA algorithm will choose the dictionary element that mostly matches the input training patch by finding the largest value of the dot product between the input and the dictionary elements. After identifying the winner neuron, the dictionary Φ_w is updated with Oja's rule, where β is the learning rate.

$$y = X^T \Phi_w \tag{3-3a}$$

$$\Delta \Phi_w = \beta (X - y \Phi_w) y \tag{3-3b}$$

After repeating Equations (3-3a) and (3-3b), the weight matrix will eventually converge to the final dictionary with learned features.



Initial weights

Dictionary after training

Figure 3-7: Device weights (dictionary elements) before (a) and after (b) training using WTA and the natural images shown in Figure 3-1. Each dictionary element is represented by the conductance values of the 16 memristors associated with the given neuron.

Figure 3-7 shows the offline training results using the memristor model on a 16×32 crossbar array, corresponding to a $2 \times$ overcomplete dictionary with 16 inputs and 32 output neurons (dictionary elements). Before training, the weights are randomly initialized, as shown in Figure

3-7a. The network is trained with 150k samples. After training is completed, receptive fields resembling Gabor filters, represented by the conductances of memristors associated with each output neuron, can be clearly observed, as shown in Figure 3-7b. No device variation effect is considered in this example.

We have also analyzed how the memristor network can implement online learning with this approach. The largest difference between the online learning case and the offline learning case is that in the offline case the receptive fields (dictionary elements) were obtained using an ideal device model and variations were only considered when the receptive fields were stored in the memristor array; while in the online learning case device variations were carefully considered during the learning stage that required large numbers of incremental weight updates.

Additionally, in the online case the same array that was trained was used for reconstructions of test images, thus dictionary storage is no longer needed. Simple single shot programming schemes (i.e. without a verify stage to check if the updated weight matches the target weight) were also used for the weight updates during the online training case.



Figure 3-8: Device weights before and after online dictionary learning A) Initial weights. B) Simulated learned weights considering device variabilities during online learning.



The model incorporating device variations during weight updates was then used to simulate online learning in the memristor crossbar. WTA based learning was first analyzed. The dictionary after learning based on WTA is shown in Figure 3-8b. As can be observed from Figure 3-8, the online learned dictioanry is very similar to the ideal case in Figure 3-7.

After learning, the same crossbar was used to process test images using the learned dictionary. Image reconstruction results using the online learned dictionary are shown in Figure 3-9. For comparison, simulation results of reconstructed images using an ideal dictionary without device variations are also included (Figure 3-7b).



Figure 3-9: Comparison of Image reconstruction with ideal dictionary and online learned dictionary (a) Reconstructed image with ideal dictionary without device variations. (b) Reconstructed image with online learned dictionary and device variations.

An interesting observation is that better results, closer to the ideal dictionary case, are obtained with the online learning process compared with results obtained from the stored, offline-learned weights, as shown in Table 3-1. This effect can be explained from the fact that the learning algorithm is self-adaptive and adjusts to the device variabilities during the training stage. As a result, online learning can more effectively handle device variations compared to the offline training and weight storage method, where the differences of specific devices was not factored into the learned dictionary and can lead to larger errors during image reconstruction, as shown in Table 3-1.

	MSE	L ₀ norm	MSE	L_0 norm	MSE	L_0 norm
Offline learning	3.579×10⁻³	11.61	1.615×10 ⁻²	9.14	7.235×10 ⁻³	5.21
Online learning	2.779×10 ⁻³	10.2	1.385×10 ⁻²	8.28	6.184×10 ⁻³	4.94
Ideal dictionary	2.224×10 ⁻³	10.68	1.065×10 ⁻²	7.88	4.866×10 ⁻³	4.83

Table 3-1: Comparison of the online and offline learning results vs. results obtained from an ideal case MSE: mean square error of the reconstructed image. L₀ norm: average number of neurons used in the reconstruction, which measures the sparsity of the image reconstruction.

3.3 Other Nonideal Effects of Experimental Constraints

In section 3.2 we demonstrated that online learning with memristor crossbar array can be successfully achieved even with device variations. To correctly train the dictionary weights, we usually use very small learning rate β (~10⁻⁵) in Equation (3-3) during simulation to guarantee gradual training during thousands of training.



Figure 3-10: Uneven training with winner-take-all in real device experiments The training tends to get stuck at certain columns

However, when implementing this approach in experiments, we found out that training tends to be uneven and concentrated at few neurons (columns) in the crossbar. Even after we remove the over-trained column, the training will keep stuck at only a few columns (Figure 3-10). To figure out the cause of this issue, we revisited our online learning strategy of winner-take-all (WTA).

3.3.1 Influence of Realistic Memristor Behaviors

We first revisit the device model in Equations (2-4), where *w* is the device state variable, γ , σ and α , λ are the tunneling and Schottky current parameters, and η_1 , η_2 describe weight update dynamics.

A main reason that causes the non-uniform training is that in realistic experiments, the programing pulse width has to be sufficiently large to initiate device weight changes (which cannot be made arbitrarily small), suggesting the actual learning rate β in Equation (3-3) will not be very small. In fact, the effective $\Delta \Phi_w = \beta (X - y \Phi_w) y$, which will be converted to programming pulsewidth during the experiments, should be around μ s to initiate ion migration. This experimental limit is equivalent to set $\Delta \Phi_w$ to be at least 10⁻⁴, corresponding to a relatively large β .

Moreover, the relatively large β will in turn amplify the device variation effects during training, especially from the following two factors:

1. Initial weight state w distribution: In realistic memristor devices, most devices have low initial state w in (2-4a), except some outliers with relatively larger conductance due to device variation, which makes those devices outweigh others and dominate during WTA analysis.

2. Variations during weight update: Another major factor that contributes uneven training is device-to-device variation during weight update. Devices with large η_1 , η_2 will have their weights grow at much faster rates than other devices.

These three factors can lead to the continued increase of conductances in a few dominant columns, resulting in the training stuck at those columns and eventually training failure^{47,48}. In practice, this problem is reflected in the networks' inability to normalize the weights to correctly produce the winning neurons, as discussed below.

3.3.2 Lack of Normalization in Winner-Take-All

In winner-take-all, we simply use the vector-matrix multiplication result to find the closest matching dictionary element, based on the distance between input *X* and dictionary element Φ_j .

$$|X - \Phi_j| = \sqrt{|X|^2 - 2X^T \Phi_j + |\Phi_j|^2}$$
 (3-4)

As can be seen from Equation (3-4), finding the minimum distance can be substituted with locating the maximum $X^T \Phi_j$, on the condition that all dictionary elements $|\Phi_j|$ are normalized.

However, in realistic memristor array, normalization of the entire matrix weight is nontrivial, since it requires calculation of the norms and update the entire array, which is computational expensive and also time consuming.

Due to the lack of normalization in the array, the dot-product results cannot accurately represent the resemblance of the input feature and the dictionary element. As a result, the columns that by chance have high conductance values will likely to win, and with the large learning rate these neurons will also receive large weight updates, causing the training to be stuck at these columns, as shown in Figure 3-11.



Figure 3-11: 50 randomly selected 7×7 dictionary elements out of 98 elements. The array is unevenly trained due to the constraints of realistic experimental conditions

3.4 Epsilon-greedy Strategy

To solve this uneven training issue, we need to take strategies to improve the uniformity of the training process, meanwhile still maintaining the simplicity of the winner-take-all learning rule of.

WTA is a so-called "greedy" algorithm, which always pick the winner of all elements. This strategy has a downside since the training can easily get stuck at some dominating elements, and end up with uneven training which only concentrated on few columns. To improve the uniformity of distribution of the outcome, we chose the epsilon-greedy strategy in this study.

Epsilon-greedy strategy is essentially a modified greedy strategy, as its name suggested. ϵ is a probability variable that indicate the proportion of randomness in the greedy approach. During the proportion 1- ϵ (i.e. the most time of the training), the greedy strategy is applied; and during the proportion ϵ , a random outcome (with uniform probability) is selected.

This epsilon-greedy strategy applies the "*exploration and exploitation*" concept in reinforcement learning⁴⁹. It does that by not only utilizing the maximum dot-product

(exploitation), but also by exploring all neurons to improve the overall decision by randomly training a column *(exploration)*, which guarantees all the devices are trained in some degree. By combining both approaches, an improved learning can be achieved.

We simulated the online dictionary learning using our realistic device model with device parameters extracted from actual devices. Training results with epsilon-greedy strategy were compared in Figure 3-12, showing similar results with an ideal dictionary learning from the same training set, and much improved compared with the WTA results in Figure 3-12. In the example given in this paper, a 49×98, 2× over-complete memristor array was initialized with a Gaussian distribution of 0.1 mean and 0.13 standard deviation. β was chosen so that the pulse widths are in several µs. η_1 and η_2 were set with 3% and 1% variations respectively. ϵ was set to be 0.1 in learning.



Figure 3-12: Comparison of 49 randomly chosen (a) ideal dictionary elements and (b) dictionary elements trained with ϵ -greedy strategy

3.5 Conclusion

In this chapter, we discussed the consequences of realistic device nonidealities on online dictionary learning. We investigated the conventional dictionary learning approach via sparse coding and stochastic gradient descent, which produced good performance but is not very hardware friendly. Instead, we developed a simpler learning approach with Oja's rule and winner-take-all. To address the nonuniform training distribution under realistic experimental constraints, an epsilon-greedy strategy was proposed. Our simulation results verified the effectiveness of the learning algorithm, which can produce desired dictionary training using simple WTA without weight normalization.

Chapter 4 Integrated Memristor-CMOS System for Neuromorphic Computing Applications

In Chapter 2, we successfully demonstrated a sparse coding hardware system in a memristor crossbar architecture. This approach, based on pattern matching and neuron lateral inhibition, is an important milestone in the development of large-scale, low power neuromorphic computing systems. The use of a crossbar architecture allows matrix operations, including matrix-vector dot-product operation and matrix transpose operations, to be performed directly and efficiently in the analog domain without the need to read each stored weight. Image reconstruction was also demonstrated using the memristor system, and online dictionary learning was shown to be feasible even in the presence of realistic device variations.

Although the key matrix operations can be performed efficiently with memristor crossbar arrays^{26,27,42}, previous implementations have largely relied on external printed-circuit boards to provide the required interface and control circuitry^{23,26,28}, or used discrete parameter analyzers to generate and collect signals^{22,24,27}. In the cases where memristor arrays are integrated with periphery circuitry, the circuit's function has been limited to providing access devices (e.g. in the form of 1T1R arrays^{23,25,26,42}) or address decoding purposes^{50,51}. To demonstrate the potential of memristor-based computing hardware would require the development of fully functional systems, where the memristor crossbars are integrated with necessary analog interface circuitry (including analog-digital converters (ADCs) and digital-analog converters (DACs)), digital buses, and ideally a programmable processor to control the digital and analog components. Integrating all necessary functions on-chip will be key to enable practical implementation of memristor-based computing systems and allow the prototypes to be scaled to larger systems.

In this chapter, we discuss our effort in building a complete neuromorphic computing system, with memristor crossbar array directly integrated on custom-designed CMOS circuitry that performs all necessary periphery, neuronal and control functions. The flexibility of the hardware system in turn allows different algorithms to be implemented on the integrated chip through simple re-programming.

4.1 CMOS Chip Overview

The integrated memristor/CMOS chip aims to demonstrate all functions, including inference and online learning, on chip, with the memristor crossbar performing weight storage and vectormatrix multiplication functions while the CMOS circuitry performing the necessary periphery functions and signal control.

The CMOS circuitry was designed by collaborators (Justin M. Correll, Dr. Yong Lim, Vishishtha Bothra and Chester Liu) from Prof. Michael Flynn and Prof. Zhengya Zhang groups. The CMOS circuitry is essentially an upgraded version of the PCB board setup used in Chapter 2. The CMOS system are capable of storing and executing C programming independently with the on chip OpenRISC core, and can apply voltage and read current at each row and column of the crossbar. This setup allows us to perform all functions of the network on chip, through the hybrid integrated memristor crossbar and the underlying CMOS circuitry.

4.1.1 System Architecture

The CMOS circuitry mainly consists of three sections (Figure 4-1):

- 1. 54 + 108 DACs and ADCs, in both row and column directions, which facilitate write and read operations in both forward and backward directions.
- 2. On-chip OpenRISC core, which is based on the version used in our previous PCB measurement setup.
- 3. Memory blocks, which include a 32k SRAM main memory for instructions and data, and two 16k ping-pong memory for large data storage.

All three major blocks are connected to a shared system bus, which can transmit data through an on-chip UART interface to external equipment such as a computer.



Figure 4-1: Layout of the CMOS chip Blocks showing 54+108 DACs and ADCs, 64k SRAM and an OpenRISC core



Figure 4-2: Chip System Architecture

The integrated memristor/CMOS chip is comprised of the digital controller and bus shown in green, the mixed-signal interface shown in red, and the memristor crossbar shown in blue. Image credit Justin M. Correll

The CMOS circuitry is schematically shown in Figure 4-2 and Figure 4-3. The on-chip processor configures the mixed-signal interface through a set of global configuration registers and performs write and read operations through digital to analog converters (DAC) and analog to digital converters (ADC).

Since the processor is mainly used for register manipulations, the reduced instruction set Alternate Lightweight OpenRISC processor (AltOR32) is used in the design to minimize area and power consumption. The SRAM is divided into 3 parts. The processor instruction and data memory are mapped to 32k of SRAM and the remaining 32k are multiplexed between two "ping-pong" memory banks (16k each) for training data buffering. The ping-pong memory banks are dual port SRAM and can be loaded externally during processing.

The custom mixed-signal interface is shown in Figure 4-3 and includes global timing generation and configuration registers, and 162 configurable channels – all can write/read to/from the Wishbone bus (the shared digital bus in OpenRISC architecture) and mapped to the OpenRISC memory space. Each channel is set to either have an ADC, or 1 of 3 DACs connected to a row or column of the crossbar. The ADC or DAC connection is set in the mode register and the type of DAC connections is set in the DAC register along with the 6b DAC pulse input. The timing generator handles both the ADC start signal and creates the duty-cycled pulse-train for the DACs.

During operation, the processor is first used to configure the mixed-signal interface by setting the configuration registers. The processor is then paused, and the control is handed off to the timing generator of the mixed-signal interface. The timing generator operates for 64 cycles during which VMM operations and memristor weight updates are performed. The control then goes back to the processor.



Figure 4-3: Mixed Signal Interface design

The mixed-signal interface is comprised of global configuration registers and timing generation shown in brown, and 162 configurable channels (shown in green) to provide input and measure output to and from each row and column of the memristor crossbar. Image credit Justin M. Correll

4.1.2 Mixed Signal Interface for Crossbar Array

The mixed signal interface is clocked at a slower speed that the OpenRISC core clock. During the Learning and Inference modes, the OpenRISC controller asserts a GLOBAL_START signal that starts the mixed signal interface. During this time, the OpenRISC processor is delayed using NOP commands, and the clocking circuit in the mixed signal interface generates the timing to control the DACs, ADCs, and crossbar connection configuration.

There are two important registers in the mixed signal interface that provide most of the critical functions on the chip: configuration register and DAC register.

A global configuration register on the chip controls the write/read mode of all the rows and columns:

MS_GBL_CFG[2]	MS_GBL_CFG[1]	MS_GBL_CFG[0]
GBL_START	ROW_MODE	COL_MODE

Table 4-1: Configuration of the global configuration register

For example, at forward pass mode, all rows are configured as DACs and all columns are configured as ADCs, so the ROW_MODE is 1 and COL_MODE is 0. At write mode, all rows and
columns are configured as DACs, so the ROW_MODE and COL_MODE are both 1.

DAC register is mainly used to configure the pulse generator (for write or read pulses) with tunable pulse widths. Each pulse generator has the ability to generate a 63-length pulse, with pulse unit width inversely proportional to the clock speed.



Figure 4-4: Global pulse generator schematic

DAC register is a 9-bit register that holds the voltage selection data and the read/write pulse durations. The lower 6 bits (DAC_REG [5-0]) specifies the pulse durations and the higher 3 bits (DAC_REG [8-6]) selects which voltage reference the DAC connects, as shown in Table 4-2. The register is loaded by the OpenRISC controller via the Wishbone bus. The DAC registers are loaded serially from their associated (addressed) memory locations.

DAC_REG	DAC_REG	DAC_REG	DAC_REG [5-0]
[8]	[7]	[6]	
VWR_H	VWR_L	VR	PULSE_DUR

Table 4-2: Configuration of the DAC register

When all the 9 bits of the DAC register are set to 0, the corresponding row/col is configured as an ADC (with ROW_MODE or COL_MODE set to 0). In this configuration, when a GLOBAL_START signal initiates, the pulse generator unit automatically enables the ADC and perform charge accumulation, controlled by the designed internal logic on the chip.

4.1.3 Four Mode Configurations on the Integrated Chip

The COMS circuit design is flexible and allows the different blocks to be configured into different modes to facilitate mapping of a complete computing model. Since there are 2 write DACs, 1 read DAC and a 13-bit ADC at each row or column, the chip can be configured in four major modes: forward pass mode, backward pass mode, forward write mode (write) and backward write mode (erase).

When performing VMM, the chip is configured at read mode (forward or backward depends on the eqaution of the multiplication). During the VMM operation, we apply a discrete-time pulsetrain input and measure the accumulated charge from each column (row). The column (row) ADCs present a 1.2V virtual ground while the row (column) DACs apply 6-bit programmable train of fixed-amplitude 0.6V "read" pulses (1.8V-1.2V). The integrating ADCs measure the collected charge over the input period.

When performing weight update, the chip is configured at write/erase mode (depending on the need of increase/decrease the weight). During the write operation, we apply discrete-time pulse-train at both rows and columns. When writing (erasing), the row (column) DACs apply 6-bit programmable train of fixed-amplitude "write" pulses (1.9V-1V) and the column (row) DACs apply 6-bit programmable train of fixed-amplitude "erase" pulses (0.1V-1V) with the same duration, which effectively generate 1.8V (-1.8V) voltage drop across the device. The idle level of both "write" and "erase" are chosen at 1V, which is the halfway of the voltage drop to provide write protection for unselected devices in the array.

The configuration of the DAC registers at four different modes and the corresponding pulse signals are shown in the tables in Figure 4-5 to Figure 4-8. The four different colors of the DAC registers (red, gray, green and yellow) reprent the corresponding 3 DACs and 1 ADC the register is used to configure.



Figure 4-5: Forward pass mode on the integrated board

The forward pass mode is used to perform VMM to update the output neurons. In this configuration, all rows are connected to the 'Read' DACs, which pulses between $1.2V(V_{VG}) - 1.8V(V_{read})$ with the input data represented by different pulse widths, and all columns are connected to 1.2V ADC virtual ground (V_{VG}). The color table lists the DAC register configuration used to control the "Read" DACs.



Figure 4-6: Backward pass mode on the integrated board

The backward pass mode is used for calculating the vector-transposed matrix multiplication. In this configuration, all columns are connected to the 'Read' DACs, which pulses between $1.2V(V_{VG}) - 1.8V(V_{read})$ with the input data represented by different pulse widths, and all rows are connected to 1.2V ADC virtual ground (V_{VG}). The color table lists the DAC register configuration used to control the "Read" DACs and ADCs.



Figure 4-7: Write mode on the integrated board

The write mode is used for programming the memristor devices to higher conductance states. In this configuration, all rows are connected to the "Write High" DACs (with range $1V(V_{Half})$ -1.9 $V(V_{High})$) and all columns are connected to the "Write Low" DACs (with range $1V(V_{Half})$ -0.1 $V(V_{Low})$). The voltage difference 1.8V of the two DACs cross the selected device is used to program the device. The color table lists the DAC register configuration used to control the "Write High" DACs and "Write Low" DACs.



Figure 4-8: Erase mode on the integrated board

The erase mode is used for programming the memristor devices to lower conductance states. In this configuration, all columns are connected to the "Write High" DACs (with range 1V(V_{Half})-1.9V(V_{High})) and all rows are connected to the "Write Low" DACs (with range 1V(V_{Half})-0.1V(V_{Low})). The voltage difference -1.8V of the two DACs cross the selected device is used to erase the device. The color table lists the DAC register configuration used to control the "Write High" DACs and "Write Low" DACs.

4.2 Test Results from the CMOS Circuitry

After the tape-out of the multi-functional CMOS circuitry, we ran serval tests to verify the basic functions of the circuits. The tests are done in two steps:

- First, we use a breadboard and some known value resistors to test the basic read functions of the circuitry, to check the linearity and performance of the on-chip ADCs. We also probe the voltage waveforms at the terminals that will be connected to the memristors with an oscilloscope, to verify the operations of read and write mode.
- After that, an extension board is designed to lead out all the memristor pad signals to a chip carrier, which is compatible with the previous 32×32 WO_x memristor array. More high-level complex functions like array readout and pattern writing is tested in this approach.

4.2.1 Verifications of Basic Functions

We first tested the ADC functions by leading the signals from the PCB to a 10k resistor on the breadboard with jumper wires. By loading a testing C program onto the chip, we can plot the ADC number (corresponding to the charge collected passing through the resistor) when varying the applied pulse width from 0 to 63, and obtained a perfect linear curve as shown in Figure 4-9, which suggests the ADC has excellent linearity vs charge.



Figure 4-9: Forward and backward read test with a 10k resistor

We also tested the configuration of the forward pass and backward pass modes. The same 10k resistor is read twice in both forward and backward directions, and the two charge-time curves are overlapped in Figure 4-9. As can be observed from the plot, both forward and backward direction ADCs function correctly and generate almost identical results.

To verify the write operations, since a fixed value resistor cannot demonstrate the programming effect, we use the oscilloscope to monitor the waveform at two terminals of the resistor.



Figure 4-10: Waveform of two set of write-read pulses pairs. Both write and read pulses have the maximum 63 pulse width.

With the oscilloscope probe on both terminals of the test resistor, we verify the function of a 63 step-long write pulse followed by a 63 step-long read pulse. While the system is set at the forward read mode, the yellow waveform probes the selected row and the green waveform probes the selected column. As shown in Figure 4-10, at the write pulses, the row voltage goes up to V_{high} (around 1.8V) and the column voltage falls down to around V_{low} , (around 0.2V) which creates a voltage drop of V_{high} - V_{low} (around 1.6V) across the device under test (DUT). Note that the actual V_{high} and V_{low} used in the memristor experiment is 1.9V and 0.1V, to create the programming voltage required by the devices.



Figure 4-11: Zoomed-in waveform of the write pulses Both write and read pulses have the maximum 63 pulse width

Figure 4-11 shows a zoomed-in waveform of the 63-step long writing pulses. As can be observed from the waveform, instead of directly modulating the pulse width, we use the number of pulses to represent the input amplitude (effectively modulating the pulse width in discrete time domain) to eliminate errors due to pulse rise and fall time.

4.2.2 Results with Extension Board and Stand-alone Memristor Array

Although we can verify some basic functions by observing the waveform output, a better approach is to connect the circuit output to real memristor devices and verify the read/write operations. An ideal approach is direct integration of the memristor onto the CMOS circuit, which will be discussed in section 4.3.

In particular, since the direct integration of memrsitor arrays on the CMOS chip is a challenging process, to separate potential issues from the fabrication process or the CMOS design it will be very useful to perform some preliminary test with a stand-alone memristor array which we already know functions properly.

Based on this idea, we designed an extension board which can interface a standalone memristor crossbar array with the CMOS chip (Figure 4-12). We lead out all output control signals generated by the CMOS chip and feed them to the extension board, which serves as a routing board

to send the control voltages to the memristor array on the chip carrier. This approach is compatible with the previous testing setup discussed in Chapter 2 and we can reuse our 32×32 memristor arrays.



Figure 4-12: Main testing board (blue) and extension board (green).

With the extension board plugged in, we can verify the programming and erasing function with a previous working memristor array. We applied 200 writing and erasing pulse to a single device on the corner of a stand-alone memristor array. Figure 4-13 shows successful gradual conductance increase and decrease obtained through signals generated and collected from the CMOS circuitry using this setup.



Figure 4-13: Pulse program and ease curve of a single memristor device on a stand-alone chip.

Moreover, since the extension board lead out 32 row and 32 column signals from the CMOS chip and connected to the socket on the extension board, we are able to verify array operations with the extension board for the 32×32 array. We verified fundamental array operations such as pattern programming and array read-out, which enabled us to write grayscale images into the array, with a couple of examples shown in Figure 4-14.



Figure 4-14: Patterns written with extension board. A 4×4 checkerboard pattern and an "M" pattern written and read out from the memristor array using the CMOS chip.

Other than simple binary patterns, with the ability of 6-bit pulse modulation that can produce pulse width from 0 to 63, we can write more complex gray-scale image correctly, using a write-verify approach. Figure 4-15 shows an example of a 40×40 grayscale Mona Lisa image written in the array. The whole image is divided into 20×20 sections and programmed sequentially in the same array. After all four sections are stored, the complete image is stitched together.



Figure 4-15: A 40×40 grayscale Mona Lisa pattern programed onto the memristor array. The original 40×40 is dissected into four sections and programmed onto the same subarray. The previous pattern is erased each time before wiring the next section.

4.3 Integrated Memristor-CMOS Chip

Our goal of this project is to directly fabricate the memristors on top of the CMOS circuitry, which allows tight integration of the VMM operations through the memristors with the neuron and control circuitry in the CMOS layer. With such a fully integrated chip, we aim to demonstrate multiple functions.

A 54×108 WO_x-based memristor crossbar was successfully fabricated on top of the CMOS circuits, performed by my collaborator Seung Hwan Lee. Figure 4-16 and Figure 4-17 are the topview images of the chip, showing the memristor array integrated on top of the chip surface, at different zoom-levels. Each row and column of the crossbar array is connected to a specific landing pad left open during the CMOS fabrication process, and then connected to the interface circuitry through internal CMOS wiring.



Figure 4-17: Zoomed-in microscopic image of the integrated chip. Inset: SEM image of the crossbar array.

The memristor crossbar array used in this work is directly fabricated on top of the CMOS circuits. First, the bottom electrode (BE) patterns with 500 nm width are defined by e-beam lithography, the 80nm think Au BEs are then deposited (with Ni/Cr adhesion layer underneath) by

e-beam evaporation and lift-off processes. Next, 300 nm of SiO₂ is deposited by plasma-enhanced chemical vapor deposition (PECVD), followed by RIE etch back to form a spacer structure along the sidewalls of the BEs. The spacer structure allows better step coverage for the WO_x switching layer and the top electrodes (TEs) at the crosspoints, and also restricts the active device regions to the flat exposed top surface of the BEs, as shown in Figure 4-18. To prevent leakage through the switching layer among adjacent devices, the switching layer is only deposited at the crosspoint regions through patterns defined by e-beam lithography. The switching layer is formed by first depositing 20nm think W through DC sputtering and lift-off processes in the e-beam patterned regions, then through rapid thermal annealing of the patterned W islands with oxygen gas at 400°C for 60s to form the WO_x switching material. Afterwards, the TEs (Pd (40 nm)/Au (90 nm)) with 500nm width are patterned and deposited by e-beam lithography, e-beam evaporation, and liftoff processes. Finally, metallization processes are performed by photolithography (GCA AS200 AutoStep) to connect the crossbar electrodes with the CMOS landing pads that are left open during the CMOS circuit fabrication process. An in-situ etch process is performed to remove the native aluminum oxide on the CMOS landing pads, followed by deposition of 800nm thick Al with DC sputtering and lift-off processes to ensure step coverage of the deeply recessed landing pads.



Figure 4-18: A cross-section schematic of the integrated chip Showing connections of the memristor array with the CMOS circuitry through extension lines and internal CMOS wiring. Inset: cross-section of the WO_x device

The integrated memristor/CMOS chip is wire-bonded onto a pin-grid-array (PGA) package (Figure 4-19) and mounted on a PCB (Figure 4-20). The PCB provides essential power signals and

the global system clock to the integrated chip. No active circuitry (DACs, ADCs, matrix switch *etc.*) are implemented on the PCB, as these functions are all provided on-chip directly. A UART-to-serial (UART: universal asynchronous receiver-transmitter) board converts the IO data from the chip into serial data and communicate a desktop computer through a USB cable.



Figure 4-19: Integrated chip after wire bonding and packaging. The chip is wire-bonded on a pin-grid-array (PGA) package, which can be plugged into a socket on the PCB board.



Figure 4-20: Testing set-up used to power and test the integrated memristor/CMOS chip. The left green board is used to filter the power signal for ADC input. The wire bonded chip is plugged into a socket on the blue PCB board on the right. The top small board is a UART-to-serial board.

The integrated WOx devices show similar I-V characteristics as standalone WO_x arrays such as those shown in Figure 1-6. It can demonstrate typical potentiation and depression curves with consecutive programming and erasing pulses, such as those in Figure 4-21 for four different devices from the integrated memristor array.



Figure 4-21: Programming and erasing memristors on chip Weight update curves from four memristor devices measured from the crossbar array in the integrated chip. The devices were programmed by 50 write pulse at 1.8V and 50 erase pulses at -1.8V, with 82µs pulse width, using the on-chip processor and the integrated DAC/ADC circuitry.

4.4 Single Layer Perceptron for Greek Letters Classification

To verify the operation of the integrated memristor/CMOS chip, we first implemented a feed-forward single-layer perceptron (SLP) network. 5×5 binary patterns are used in the SLP training and testing.

The SLP has 26 inputs (corresponding to the 25 pixels in the image and a bias term) and 5 outputs, with the input and output neurons fully connected with $26 \times 5 = 130$ synaptic weights. The weighted sums are then calculated with a nonlinear activation function --- the classical "Softmax" function (will be discussed later). The final output values of the neurons are in the range $0 \sim 1$,

where the neuron with the highest output is identified as the winner and used to classify the corresponding class, as schematically shown in Figure 4-22.



Figure 4-22: Implementation of the SLP using a 26×10 memristor array through the integrated chip. a. Schematic of the single-layer perceptron for classification of 5×5 images. b. The input data (e.g. Greek Letter ' Ω ') are converted to voltage pulses of V_{read} or 0 through circuitry, depending on the pixel value.

In this experiment, the original binary input patterns are converted into input voltage pulses through the integrated processor and DAC circuitry and are fed to the rows of the memristor array. Specifically, when a white pixel is present, a pulse is applied to the corresponding row; while black pixels correspond to no pulse. The bias term is fixed at a constant value of 1 (treated as a white pixel) and is applied as an extra input. All the input pulses have the same duration and amplitude in this test, as illustrated in Figure 4-22.

Each synaptic weight w_{ij} is implemented with two memristors representing a positive and a negative weight, G_{ij}^+ and G_{ij}^- , respectively, using the positive memristor conductance values. The charge collected at an output neuron *j* is determined as:

$$Q_j = \sum_i w_{ij} x_i = V \sum_i G_{ij} t_i = V \sum_i (G_{ij}^+ - G_{ij}^-) t_i = Q_j^+ - Q_j^-$$
(4-1)

Where x_i is the input at row *i* and represented by a voltage pulse with amplitude *V* and width t_i . The charges are measured at the output columns and digitized by the ADCs, then converted to the neuron output y_i through the Softmax function:

$$y_j(Q_j) = \frac{\exp(\beta Q_j)}{\sum_k \exp(\beta Q_k)}$$
(4-2)

where β is a scaling number of the ADC output and k represents the output neuron index

The integrated chip allows us to perform online learning. Specifically, the synaptic weights are updated during the training state using the batch gradient descent rule:

$$\Delta w_{ij} = \eta \sum_{n=1}^{N} \left(t_j^{(n)} - y_j^{(n)} \right) x^{(n)} \tag{4-3}$$

where $x^{(n)}$ is the *n*th training sample of the input dataset, $y^{(n)}$ is the network output and $t^{(n)}$ is the corresponding label, η is the learning rate. The update value Δw_{ij} for the *i*th element in the *j*th class is then implemented in the memristors by applying programming pulses through the write DACs with a pulse width proportional to the desired weight change (quantized within the range of 0~63 timesteps, i.e. corresponding to 6-bit precision).

The SLP is mapped on the integrated chip using a 26×10 subarray. We trained and tested the SLP with noisy 5×5 Greek Letter patterns, for 5 distinct classes: ' Ω ', 'M', ' Π ', ' Σ ', ' Φ '. For each Greek letter, we flip one of the 25 pixels of the original image and generate 25 noisy images. Together with the original image they form a set of 26 images for each letter. We randomly select 16 images from the set for each class for training and use the other 10 images for testing. An example of the training set and testing set is shown in Figure 4-23 and Figure 4-24. This approach guarantees that the training set and the testing set do not overlap, and therefore improves the robustness of our testing results, since the noisy test images are not used to train the network.



Figure 4-23: Noisy training data set for the SLP.

The training data set for each class includes the original image and 15 out of the 25 noisy images created by flipping 1 pixel in the original image.



Figure 4-24: Noisy testing data set for the SLP. The testing data set includes the 10 noisy images not in the training set, created by flipping 1 pixel in the original image for each class.

Training and testing results from the experimentally implemented SLP are shown in Figure 4-25 and Figure 4-26. After 5 online training epochs the SLP can already achieve 100% classification accuracy for both the training and testing sets. The average activation of the correct neuron during training is also clearly separated from the others, and the difference in neuron outputs between the winning neuron and the other neurons improves during training, as shown in Figure 4-25, verifying online learning has been reliably implemented in the experimental setup. Compared with earlier SLP implementations²² that used the Manhattan rule and required on average 23 epochs to achieve perfect classification for a similar database, batch gradient descent used here not only considers the direction of the weight update (which is the case with the Manhattan rule), but also the value of weight update, so that much faster training convergence can be obtained, as shown in Figure 4-26.



Figure 4-25: Evolution of the output neuron signals during training, averaged over all training patterns for a specific class



Figure 4-26: Misclassification of the training and testing data set vs training epochs. The network can achieve 100% classification for both the training set and the testing set after 5 training epochs.

4.5 Sparse Coding Implementation

The same hardware system was then used to implement a sparse coding algorithm. Following our previous work implemented at the board level²⁸, we mapped the *Locally Competitive Algorithm* (*LCA*)⁴⁰ on our integrated memristor/CMOS chip.

With this approach, the LCA algorithm can be implemented in an iterative process through two vector-matrix multiplication operations; in forward direction to obtain the neuron activations, and in backward direction to obtain the reconstructed input. The residue term is then obtained by removing the reconstructed input from the original input, and is then fed to the network, and the process is repeated until the network stabilizes. Figure 4-27 illustrates the iterative forward and backward processes employed in the LCA implementation.



Figure 4-27: Schematic of the LCA algorithm using integrated chip. In each iteration a forward pass is performed to update the membrane potential u of the output neurons based on the inputs, followed by a backward pass to update the residual r based on the neuron activities a. The residual r term forms the input for the next iteration.

The bi-directional operation of the memristor array in the integrated memristor/CMOS chip allowed us to experimentally implement the sparse coding algorithm on chip. Similar to the SLP case, we use the crossbar array to perform VMM operations, here in both forward and backward directions. Since the chip offers full flexibility to implement different algorithms by reprogramming the integrated processor, the LCA algorithm was implemented in the same chip used in the SLP study, through simple software changes.

 4×4 inputs were used to test the experimental implementation of the LCA algorithm. By using linear combinations of horizontal and vertical bar patterns, the input dimension is reduced to 7. To satisfy the over-completeness requirement of the LCA algorithm, a dictionary containing 14 features of horizontal and vertical bar patterns are used, as shown in Figure 4-28a. This setup produces a $2\times$ over-complete dictionary⁴⁰ that enables the network to find a sparse, optimal solution out of several possible solutions.



Figure 4-28: Experimental demonstration of sparse coding using the integrated memristor chip a) Dictionary elements based on horizontal and vertical bars. b) The original test image. c) The experimentally reconstructed image based on the neuron activities from the memristor chip. d) Experimentally obtained neuron membrane potentials as a function of iteration number during LCA analysis. The red horizontal line marks the threshold parameter λ .

The LCA algorithm was mapped to a 16×14 subarray in the memristor/CMOS chip, using the integrated corresponding interface circuitry and the processor that provide the neuron functions. An example of the LCA network operation is shown in Figure 4-28 (b-d). The experimentally implemented network correctly reconstructs the input image while minimizing the number of activated neurons. For example, it identifies the optimized solution with two neurons 6 and 13, instead of using three neurons 2,4 and 6. Examining the dynamics of the network operation also verified the successful LCA implementation. As shown in Figure 4-28d, all neurons are charging up in the first 4 iterations. At the 5th iteration, neuron 13 first crosses the threshold, since it consists of two horizontal bars and results in a larger output value in the membrane potential update. As a result, the lateral inhibition effect in the system suppresses the membrane potentials of other neurons (2 and 4) sharing part of the patterns with neuron 13, even though they also represent features of the input. Meanwhile neuron 6 which represents the vertical bar feature continues to charge up. At iteration 11, neuron 6's membrane potential crosses the threshold and all other neurons' membrane potentials are suppressed below the threshold, leading to the finding of the optimal solution. The neurons' membrane potentials continue to evolve but those of neuron 6 and 13 remain above the threshold and those of other neurons continue to decrease due to the inhibition term and the leaky term in the membrane potential equation, and the solution from the network was read out after 30 iterations.

To verify the system's performance for other input patterns, an exhaustive test of all 24 possible patterns consisting of two horizontal bars and 1 vertical bar was performed using the onchip memristor network, resulting in 100% success rate (Figure 4-29) measured by the network's ability to correctly identify the sparse solutions.



Figure 4-29: Additional examples of input images and reconstructed images. The same threshold λ = 18 is used in all images.

4.6 Principal Component Analysis with Bilayer Networks

Finally, we demonstrate a bilayer neural network using two subarrays in the same memristor crossbar, implementing unsupervised and supervised online learning to achieve feature extraction and classification functions, respectively. The bilayer network is used to analyze and classify data obtained from breast cancer screening based on principal component analysis (PCA). Specifically, the first layer of the system is a 9×2 network that performs PCA of the original data, which reduces the 9-dimensional raw input data to a 2-dimensional space based on the learned principal components (PCs). The second layer is a 3×1 SLP layer (with differential weights and a bias term) which performs classification using the reduced data in the 2-dimensional space for the two classes (benign or malignant). The schematic and crossbar implementation of the bilayer network is shown in Figure 4-30.



Figure 4-30: Implementation of the bilayer network on the integrated chip a) Schematic of the bilayer neural network for PCA analysis and classification. b) The bilayer network is mapped onto the integrated memristor chip, using a 9×2 subarray for the PCA layer and a 3×2 subarray for the classification layer

PCA reduces data by projecting them onto lower dimensions along principal components, with the goal of finding the best summary of the data using a limited number of PCs⁵². The conventional approach to PCA is to solve the eigenvectors of the covariance matrix of the input data, which can be computationally expensive in hardware. A more hardware-friendly approach is to find the PCs through unsupervised, online learning.

Specifically, following our previous study³⁰, Sanger's rule, also known as the generalized Hebbian algorithm, is implemented in the integrated chip to obtain the PCs. The desired weight change for the j^{th} principal component is determined by:

$$\delta g_{ij} = \eta y_j \left(x_i - \sum_{k=1}^j g_{ij} y_j \right) \tag{4-4}$$

4.6.1 Mapping memristor conductance to synaptic weight in PCA

In the experiment, the weights of the 1st and 2nd PCs, g_{ij} , are mapped onto the memristor conductances through a linear transformation with range ([-1 1]), by using the relationship:

$$g = \frac{ADC - a}{b} \tag{4-5}$$

where ADC is the unconverted ADC output from the circuit, which is converted to the current/conductance value through factors *a* (ADC shift factor, which is about 1900) and *b* (ADC scaling factor, which is about 1500) in Equation (4-5). The conversion based on Equation (4-5)

maps the maximum average current to weight 1 and minimum average current to weight -1.

For each input data, the dot-product of the input data and the *j*th feature, y_j is directly obtained from the ADC output of the j_{th} column of the 9×2 weight matrix. The column's weights are then updated from the Sanger's rule in Equation (4-4)

During training, the desired weight updates are linearly converted into write pulse widths and applied to the memristor devices, without using nonlinear compensation schemes such as the one discussed. Device nonidealities including the nonlinear weight updates (as shown in Figure 4-21) caused the experimentally obtained training results to differ from the software results.

4.6.2 Training the 1st Layer for Principal Component Analysis

The network is trained online, using a subset of the original database consisting of 100 data points. During the training process, the 9-dimensional breast cancer data is converted into input voltage pulses with pulse widths proportional to the data values, within the range of 0~63 time units. The output charge collected at column *j* then corresponds to the dot-product of the input vector and the conductance vector stored in column *j*, projecting data from the original 9-dimensional space to a 2-dimensional output space (when only two principal components are used). During training, the weights are then updated following Equation (4-4), using programming voltage pulses generated through the write DACs with pulse widths proportional to δg_{ij} .

Initially, the weights of the 1st and 2nd components are randomized in the memristor array (Figure 4-31a). Projection of the input along these vectors leads to severe overlapping of the benign and malignant cases in the 2-dimensional space, as shown in Figure 4-31b and Figure 4-31c. After 30 training epochs (an epoch is defined as a training cycle through the 100 training data), the PCs are correctly learned (Figure 4-32a), and the 2-dimensional projected data can be clearly separated into two clusters, as shown in Figure 4-32b and Figure 4-32c. Note the ground truth (benign or malignant) is not used in the PCA training or clustering process. They are included in the plots (represented as blue and red colors) only to highlight the effectiveness of the clustering before and after learning the PCs.



Figure 4-31: Weight and data distribution before PCA. a) Initial weights for the two PCs in the network. Before training, linear separation is not possible in the projected 2-dimenstional space, for both training (b) and testing data (c).





a) Weights for the two PCs after unsupervised, online training obtained from the memristor network, using Sanger's learning rule for 30 cycles of training. Clear separation can be observed in the 2dimenstional space for both training (b) and testing (c) data after projection along the trained PCs.

The PCA layer separate the original data into clusters, but does not classify them. To achieve classification, we implemented a second layer, a SLP, in the same hardware system. The on-chip DACs offer 6-bit resolution and can generate pulses of range 0~63. However, after the PCA process, the 2-D projected data have analog and negative values. To use the PCA output data as input to the second, perceptron layer, we need to rescale the data to the range of 0~63 and quantize them into pulse numbers.

4.6.3 Scaling of the PCA layer output as perceptron layer input

As can be observed from Figure 4-32, most of the PCA output data are located in the range of $3\sim25$ in the x axis and $-15\sim3$ in the y axis. To quantize and scale the data to the range of $0\sim63$ for the perceptron layer, the following formulas are used:

$$\hat{x} = round[2x] \tag{4-6a}$$

$$\hat{y} = round[-3(y-3)]$$
 (4-6b)

Notice that some outlier data points would produce values larger than 63. These few points were mapped to 0 pulses so that all other points can make use of as much dynamic range of 0~63 as possible.

After quantization and scaling, the data are classified using the perception layer, and the results are shown in Figure 4-33. The labels are directly obtained from the neuron outputs in the perceptron layer, without reading the weight values. Finally, data were replotted in the original PCA output space, using the obtained corresponding label for each data point, as shown in Figure 4-34.



Figure 4-33: Classification of the quantized data.

Outputs from the PCA layer were quantized and scaled to the range of 0~63, and used as input to the second perceptron layer. The quantized data were then classified by the perception layer, with blue points representing the network classified benign data and red points representing the network classified malignant data.



Figure 4-34: Replotted classification results in the original space. The classified results in Figure 14 were then replotted in the original output space from the PCA layer, with blue points representing the network classified benign data and red points representing the network classified malignant data.

4.6.4 Training of the 2nd perceptron layer for classification

The SLP processes outputs from the PCA layer and generates a label (benign or malignant). Since there are only two classes to distinguish, the SLP is trained online using logistic regression. A 3×2 subarray is used in the second layer, to account for the 2 inputs, the bias term, and the differential weights.

The training rule based on logistic regression using batch gradient descent has a similar format as the Softmax regression used in Equation (4-7):

$$\Delta w_i = \eta \sum_{n=1}^{N} (t^{(n)} - y^{(n)}) x_i^{(n)}$$
(4-7)

where η is the learning rate, $y^{(n)}$, $t^{(n)}$, $x^{(n)}$ are the neuron outputs, ground truth label and input data for the n^{th} input sample.

After learning the PCs in the PCA layer, the original 9-dimensional data are fed through the PCA layer, and the clustered 2-dimensional data are used as inputs for the SLP layer. The same 100 training data used for the PCA layer training are used for the SLP layer training (Figure 4-35), in a supervised fashion using the ground truth (the label associated with the original data). Training is completed after 30 epochs.



Figure 4-35: Evolution of the number of misclassifications during the online training process

Afterwards, the 500 test data not included in the training set are applied to the network, passing first through the PCA layer then as 2-dimentional data into the 2nd SLP layer. After online training of the PCA and the SLP layers, the experimentally implemented 2-layer network can achieve 94% and 94.6% classification accuracy during training and testing (Figure 4-36). The values are slightly lower than the ones obtained from software implementation (95% during training and 96.8% during testing, Figure 4-37), due to the nonideality in the memristor weight update that results in a decision boundary that differs from that obtained from software (which assumes ideal linear weight updates) after the online training process. We expect future device optimizations that can improve device weight update linearity^{25,53} will further improve the network performance and enable large scale practical hardware implementations.



Figure 4-36: Classification results experimentally obtained from the memristor chip. The blue and red colors represent the predicted benign and malignant data, respectively. The incorrectly classified results are marked as hollow circles. Classification rates of 94% and 94.6% are obtained for the training (a) and testing (b) data, respectively



Figure 4-37: Classification results of the bilayer network implemented in software. The blue and red colors represent the predicted benign and malignant data, respectively. The incorrectly classified results are marked as hollow circle. Classification rates of 95% and 96.8% are obtained for the training (a) and testing (b) data in software, respectively.

4.7 **Power Analysis and Estimation**

The power consumption of the integrated memristor/CMOS system consists of three parts: the digital OpenRISC core, the mixed signal interface, and the power consumed by the passive crossbar array.

Both the digital processor power and mixed signal interface power are directly measured experimentally, by measuring the root mean square (RMS) current with a Fluke meter while running the chip, with the help of Justin M. Correll from Prof. Michael P. Flynn's group. At the maximum frequency of 148MHz, the digital power reads 235.3mW and the total analog power reads around 64.4mW. The crossbar array power is obtained from the average device current at the read voltage, which yields ~7mW for the 54×108 array. The total power at 148MHz clock is thus 306.7mW for the current chip based on 180nm CMOS technology.

The energy efficiency is estimated using the 148MHz clock speed and an average 4-bit input during inference, which gives around 9.4M VMM operations per second. Multiplying this number by 54×108 lead to 5.48×10^{10} operations per second. Therefore, the energy efficiency can be derived by dividing the number of ops/second with the total power, which results in 178.68 GOPS/W for the current memristor/CMOS chip.

The custom circuitry was designed in 180nm CMOS and features a generic digital processor along with a full set of mixed signal analog to digital converters (ADC) and digital to analog converters (DAC). Two different approaches were used to estimate the power dissipation at the 40nm technology node. The digital power was estimated using generalized scaling⁵⁴ and the mixed-signal power was estimated using a figure of merit (FOM) approach.

In digital circuits, the length scaling factor S, and the supply voltage scaling factor U are different during scaling. We chose the generalized scaling approach for digital power.

Specifically, from 180nm to 40nm, S = 180nm/40nm = 4.5, U = 1.8V/1.0V = 1.8. As a result, the digital power is reduced by a factor of $1/U^2 = 0.32$, while the circuit speed is improved by a factor of S = 4.5. Note the faster processor allows the same process to control more channels, so normalizing to the same number of 162 channels, the digital power at 40nm is estimated to be

$$P_{40nm} = \frac{P_{180nm}}{U^2 S} \tag{4-8}$$

Using the measured digital power at 180nm, the estimated digital power at 40nm is then

235.3mW/((1.8)²×4.5), which is about 16.1mW.



Figure 4-38: Schreier FOM for 180nm and 40nm ADCs published in ISSCC and VLSI conferences from 1997-2018. The Schreier FOM is used for comparing high-resolution ADC performance across architectures. Image credit: Justin M. Correll

The analog to digital converter performance is evaluated using various figures of merit (FOM). An ADC FOM combines several converter performance metrics into one number for comparison across ADC architectures. The Schreier FOM is typically used for high-resolution converters and is given by the following equation:

$$FOM_s = SNDR + 10\log\left(\frac{BW}{P}\right)$$
 (4 - 9)

where *SNDR* is the signal to noise ratio and distortion, *BW* is one-half of the sampling frequency, and *P* is the power dissipation. To estimate the power scaling from 180nm to 40nm, the ADC Performance Survey⁵⁵ was used which aggregates all ADCs published in the ISSCC and VLSI circuits conferences from 1997 - 2018. A subset of data for 180nm and 40nm ADCs is shown in Figure 4-38. The mean FOM between sampling frequencies from 100kHz to 10MHz for each technology was determined and compared. The mean FOM for 40nm was determined at 172dB and a conservative estimate of 165dB was used for power estimation. Using an estimated 165 dB,

which corresponds to 176µW per ADC, we can get the new total analog power at 40nm is 19mW, leading to a total system power of 42.1mW, assuming the 54×108 crossbar power remains at 7mW. Therefore, by simply scaling the system to 40nm technology node, the estimated OPS/W at 148MHz is 1.3TOPS/W. The power efficiency can be further improved by further scaling the CMOS circuit to more advanced technology nodes. Additionally, the digital power can be further improved by using a more custom controller design instead of using a generic processor, while the analog power can be improved by further optimizations of the ADC circuitry (e.g. replacing the fast and high-precision 13-bit ADC with simpler interface circuits), along with memristor device optimizations to reduce the crossbar power.

4.8 Conclusion

In this chapter, we successfully designed and fabricated a fully-functional, programmable neuromorphic computing chip with a passive memristor crossbar array directly integrated with a complete set of analog and digital components and an on-chip processor. The integrated chip allows mapping of different neuromorphic and machine learning algorithms on chip through simple software changes. Three different and commonly-used models, perceptron, sparse coding and principal component analysis with an integrated classification layer, were demonstrated. 100% classification accuracy was achieved for 5×5 noisy Greek Letters in the SLP implementation, reliable sparse coding analysis was obtained from an exhaustive test set using 4×4 bar patterns, and 94.6% classification rate was experimentally obtained from the breast cancer screening dataset using the same integrated chip.

The integrated chip suggests different computing tasks can be efficiently mapped on the memristor-based computing platform, by taking advantage of the bidirectional VMM operations in the memristor crossbars and the flexibility in the CMOS interface and control circuitry. In our prototype, the supporting analog interfaces, as well as digital control and the OpenRISC processor are implemented in 180nm CMOS technology.

The entire mixed-signal interface with independent ADCs and DACs supporting the 54×108 crossbar and operating at the maximum frequency of 148 MHz consumes 64.4 mW from the experimental measurements. This corresponds to energy consumption of 27.4 nJ/inner product or 4.7 pJ/op for the mixed-signal interface, where an operation is defined as the multiplication and

accumulate (MAC) process of a 4-bit input with a stored analog weight in the memristor array. At the maximum operating frequency of 148 MHz, the total system power of 306.7 mW and a power efficiency of 178.68 GOPS/W for the experimentally demonstrated memristor/CMOS chip based on 180 nm CMOS technology. Simply scaling the design to a more advanced process node such as 40 nm CMOS technology the power efficiency 1.3 TOPS/W can be achieved. We believe further optimizations of the system design, e.g. by replacing the generic processor with a custom-designed controller, and by replacing the fast and high-precision 13-bit ADC with simpler interface circuits, along with memristor device optimizations that reduce power consumption in the memristor crossbar, can further improve the system's performance and power efficiency.

Chapter 5 Reservoir Computing with Memristor Devices

The previous studies from Chapter 2 to Chapter 4 mainly focus on using memristor crossbar structures to act as a matrix operation accelerator to implement neural network applications such as sparse coding or feedforward networks. However, dynamic memristor behaviors discussed in Chapter 1 can also be used to natively perform other computing tasks. One interesting and important application is reservoir computing (RC), where the short-term memory effect of memristors can be utilized for efficient temporal information processing.

In this study, we experimentally demonstrate a memristor-based RC system using dynamic memristor devices that offer internal, short-term memory effects^{17,56,57}. These dynamic effects allow the devices to map temporal input patterns into different reservoir states, represented by the collective memristor resistance states, which can then be further processed through a simple readout function. The memristor-based RC hardware system is then used to experimentally perform hand digit recognition tasks and solve a 2nd-order nonlinear task.

5.1 Reservoir Computing

Reservoir Computing (RC) is a novel neural network-based computing paradigm that allows effective processing of time varying inputs^{58–60}. An RC system is conceptually illustrated in Figure 5-1, and can be divided into two parts: the first part, connected to the input, is called the *reservoir*. The connectivity structure of the reservoir will remain fixed at all times (thus requiring no training), however, the neurons (network nodes) in the reservoir will evolve dynamically with the temporal input signals. The collective states of all neurons in the reservoir at time *t* form the reservoir state x(t). Through the dynamic evolutions of the neurons, the reservoir essentially maps the input u(t) to a new space represented by x(t) and performs a nonlinear transformation of the input. The different reservoir states obtained are then analyzed by the second part of the system, termed the *readout function*, which can be trained and is used to generate the final desired output y(t). Since training a RC system only involves training the connection weights (red arrows in the

figure) in the readout function between the reservoir and the output⁶¹, training cost can be significantly reduced compared with a conventional recurrent neural network (RNN) approaches⁶¹



Figure 5-1: Schematic of an RC system, showing the reservoir with internal dynamics and a readout function

The readout function in an RC system is typically simple (thus easy to train) and is normally based on a linearly weighted combination of the reservoir neuron node values. As a result, it is memory-less. To process temporal information, the reservoir state needs to be determined not only by the present input but also by inputs within a certain period in the past. Therefore, the reservoir itself must have short-term memory. In fact, it has been mathematically shown⁶⁰ that a RC system only needs to possess two very unrestrictive properties to achieve universal computation power for time-varying inputs: point-wise separation property for the reservoir, which means that all output-relevant differences in the input series $u_1()$ and $u_2()$ before time *t* are reflected in the corresponding reservoir internal states $x_1()$ and $x_2()$ that are separable; and approximation property for the readout function, which means that the readout function can map the current reservoir state to the desired current output with required accuracy.

5.2 Short-term Memory WO_x Memristor as Reservoir

In this study, memristor devices with short-term memory effects^{17,56,57} were used to act as the reservoir in an RC system. During device fabrication, the switching layer of the WO_x based device was specifically designed to exhibit short-term memory (*i.e.* volatile) behavior^{17,56,57}

To demonstrate the temporal dynamics of the device, a pulse stream composed of write pulses having the same amplitude (1.4 V, 500 μ s) but at different timeframes are applied to the

device and the response of the memristor, which is represented by the read current through a small read pulse (0.6 V, 500 μ s) following each write pulse, is recorded. The results are shown in Figure 5-2.



Figure 5-2: Memristor's temporal response to a pulse train. Write pulses (1.4 V, 500 μ s) with different timing (blue lines) were applied and the response, represented by current measured by a small read pulse (0.6 V, 500 μ s) after each write pulse is recorded. A temporal response is observed.

Two properties, similar to results obtained in dynamic synapses, can be observed:

(1) If multiple pulses are applied with short intervals, the response will gradually increase (as indicated by the red arrow in the figure), showing an accumulation effect

(2) If there is a long enough period without any stimulation, then the device state will decay towards the original resting state, as indicated by the green arrow in the figure. This temporal response is attributed to the internal ionic processes of the WO_x memristor, including the drift under electric field during the spike and the spontaneous diffusion of oxygen vacancies after the spike, and can be well modeled within the memristor theoretical framework^{17,56,57,62}.

The memristor's short-term memory effect can be described by a time constant τ , and for devices used in this study is ~ 50ms. As a result, when programming the device, the device state depends not only on the programming pulse itself, but also depends on whether other programming pulses have been applied in the immediate past within a period of ~50ms. Prior programming

pulses applied within this range will affect the device state, with pulses applied closer to present time having a stronger effect, while events happened much earlier will not affect the present device state since the device would have decayed to the initial state already.

The short-term memory effect of the memristors allow the device to natively implement the "fading memory" property of the reservoir, without having to constructing loops in the network. Based on this concept, we performed experimental studies on RC using memristors in a crossbar array.

The 32×32 WO_x memristor array was fabricated with 500nm line width by Dr. Chao Du, as shown in Figure 5-3, and wire-bonded to a chip carrier and mounted on a customized board for testing. We select the 90 devices from the array for the RC studies in a way to avoid having adjacent devices in both row and column direction to minimize the write disturbance.



Figure 5-3: Experimental setup for RC.

32x32 WOx memristor array fabricated. 5 cells from the array are used as the reservoir.

To verify the operation of the devices in the array, we send the same pulse streams to all the 90 devices individually and measure the device response. We found out that besides expected device to device variations, all devices can response to the input pulse sequence correctly and demonstrate similar current dynamics. The response to 4 different pulse squences from all 90 devices are shown in Figure 5-4.


Figure 5-4: Response from the 90 devices to four different input pulse sequences. All devices demonstrate similar response to the input pulse streams.

To verify that a unique input sequence will always lead to the same output, we performed a test where one memristor device in the reservoir is repeatedly tested, while the other devices remain unperturbed. In this case, since all other devices remain unchanged, the reservoir state can be represented by the resistance value of the device that is being stimulated. As seen in Figure 5-5, the same input sequence always leads to the same unique device response (and thus the overall reservoir state).



The device shows similar response to each input pulse stream.

To further verify the separation property of the memristor-based reservoir for unique input signals, we tested the memristor's response to all possible combinations of length-4 pulse streams, shown in Figure 5-6. A different memristor state (as reflected by the read current after the pulse stream) was obtained for each pulse stream input, indicating that the memristor can separate those ten different pulse stream patterns.



Figure 5-6: Memristor's response to ten pulse trains. Ten pulse trains corresponding to ten different row pixel arrangements for the ten digit images were input to a memristor and the read currents after the forth pulse show ten different levels that can be well-separated.

5.3 Reservoirs Computing for Digit Recognition

5.3.1 Training and Classification of 4×5 Digit Images

To test the functionality of our memristor reservoir, we start with a simple task by processing computer generated images. The task is to recognize the digit from a 4×5 input image, which has 20 pixels, either black ("0") or white ("1"). For the 10 digits represented by the 4×5 images shown in Figure 5-7.



Figure 5-7: Simple digit images. Each digit image contains twenty pixels, either black or white.

Take digit "2" as an example. It is then divided into 5 rows, each row containing 4

consecutive pixels and is fed into a memristor in the reservoir as a 4-timeframe input stream. A timeframe (3 ms in width) will contain a write pulse (1.5 V, 1 ms) if the corresponding pixel is a white pixel, or no pulse (equivalently a pulse with amplitude of 0 V) if the corresponding pixel is a black pixel⁶³. Therefore, information of the image for digit "2", which is represented by the spatial locations of the white pixels in each row, is represented by temporal features streamed into the reservoir, *i.e.*, a pulse stream with pulses applied at different timeframes. The goal is to extract information of the image, *i.e.* the digit number 2 here, by collectively processing the temporal features in the 5 input pulse streams. Here only 5 memristors were used to process the image, with each memristor processing the input pulse stream from a specific row in the image. The reservoir state is represented by the collective resistance states of the 5 memristors. After the application of the input streams, the reservoir state is thus dependent on the input temporal patterns and can be used to analyze the input (Figure 5-8).





Specifically, when a pulse is applied, the state of the memristor will be changed (reflected as a conductance increase) and if multiple pulses are applied with short interval a larger increase in conductance will be achieved, while long intervals without stimulation will result in the memristor state (conductance) decaying towards its resting state, *i.e.*, the initial state before any pulse is applied. Therefore, different temporal inputs will lead to different states of the device and consequently the overall reservoir state. In this specific setup, each memristor's state after stimulation will thus represent a specific feature for the given row in the original image, and the collective device states, representing the reservoir state, can be used to perform pattern recognition

through the (trained) readout function, *i.e.* identifying the digit as "2" of the original input (Figure 5-8).

The readout function here is a 5×10 network, with the reservoir state, measured by the read currents from the 5 memristors in the reservoir, as the input, and 10 output neurons (labeled 0-9) representing the predicted digit value of the input image, schematically illustrated in Figure 5-9. During classification, the output from the 10 output neurons are calculated from the dot product of the 5 inputs and the weights associated with each output neuron, and the output with the maximum dot product is selected and its label number is used as the predicted digit value. The readout function is trained in a supervised fashion based on Softmax regression (explained with details in Chapter 4) where the weights are adjusted to minimize output error during training.

Figure 5-9 shows the reservoir state, represented by the combination of the 5 memristors' resistance values, after feeding the reservoir with the 10 images shown in Figure 5-7. The reservoir states are significantly different, verifying the reservoir's ability to clearly separate these 10 cases.



Figure 5-9: Liquid's internal states after subjected to the ten digit inputs. The read currents of the 5 memristors were recorded as the internal state of the liquid and significant differences can be observed.

The reservoir state was then used as input to the readout network for training and classification. After 200 training iterations, the RC system can correctly recognize all inputs from the 10 original images. To test the effects of cycle-to-cycle variations of the device, the 10 images were repeatedly tested ten times without retraining the readout function, and 100% accuracy was verified experimentally in the memristor-based RC system for this simple task.

5.3.2 Training and Classification of Hand Written Images

Following these demonstrations, the memristor-based RC system was then tested with a more complex, real-world task, that is, recognition of handwritten digits. We train and test the system with the commonly used Mixed National Institute of Standards and Technology database $(MNIST)^{64}$. A preprocessing was performed before the images were fed into the reservoir, as shown in Figure 5-10. Take the image of digit "8" as an example, the original grayscale image was first converted into a binary-pixel image. The unused boarder area was also removed to reduce the original 28×28 image into a 22×20 image with 22 rows and 20 pixels per row. Some of the preprocessed samples from MNIST are shown in Figure 5-10.



Figure 5-10: Samples from the MNIST database.

Since the original images of the MNIST is 28x28 grayscale images, optimization methods were introduced to improve the ability of the reservoir to separate the inputs.

- The original grayscale image was first transformed into a binary-pixel image. The unused boarder area was removed by reducing the original 28×28-pixel image into 22×20. For each row, there are now 20 pixels.
- 2. Each row is divided into smaller sections (*e.g.* 4 sections with each section now containing 5 pixels) to allow better separation of the inputs.
- 3. The same input as pulse streams is applied at different rates (by using different timeframe widths). The rational is as follows. If the timeframe is short and thus the interval between pulses is small (compared to the decay time constant of the memristor), the increased conductance caused by each pulse will not decay much before the next pulse arrives. As a result, the final memristor conductance is largely

determined by the number of pulses in the input due to the cumulative effects of the conductance increases.



Figure 5-11: LSM for handwritten digit recognition.

Image of the digit was preprocessed and transformed into pulse trains. Then pulse trains with different temporal patterns were input to the liquid with different rates. With a trained readout, the recognition results will be obtained.

With these considerations, the image is fed into the reservoir in 5 pixel sections as input pulse streams and applied with two different rates, as shown in Figure 5-11. The readout network is trained using Softmax regression as discussed earlier. 14000 images from the MNIST data set were used for the readout function training. After training, another set of samples consisting of 2000 images not in the training set, are used to test the recognition accuracy. The reservoir state was then fed to the readout function to perform classification. In the experimental study, 88 memristors were used as the reservoir (22 rows, 4 sections and 2 rates), and a 176×10 readout network was used for classification. From the 2000 test images, an 88.1% accuracy was obtained from the RC system.

The memristor-based RC system was further analyzed through simulation using a physicsbased memristor model. From simulations based on the dynamic WO_x memristor model¹⁷, an RC system with a reservoir consisted of 88 memristor devices (22 rows, each row has 4 sections and each section is input at 2 rates) can potentially achieve 91.1% recognition accuracy. Increasing the reservoir to 112 memristors (28 rows, 4 sections, 3 rates) improves the performance slightly to 91.5% accuracy (More results are shown in Table 5-1). The lower accuracy obtained in the experimental network can be attributed to the cycle-to-cycle variations of the device response, during training and image analysis stages. We note that even with these non-idealities, the experimental results, with a much smaller network and dealing with a simplified, truncated input, are already better than the 88% accuracy achieved previously by simulation based on a one-layer neural network with 7850 free parameters, using pixel values of the entire digit image as the input⁶⁵.

	Data Preprocessing	Number of samples	Sections of Each Row	Rates	Recognition Accuracy (%)
Simulation	Initial images 28×28	Training: 60000 Test: 10000	4	3 horizontal + 3 vertical	92.1
				3	91.5
				2	91.0
				1	86.0
	Truncating initial image size to 22×20	Training: 60000 Test: 10000	4	2	91.1
				1	88.2
			2	2	89.0
				1	79.9
Experiment	Truncating initial image size to 22×20	Training: 14000	4	2	88.1
		Test: 2000		1	85.6

Table 5-1: Experimental and simulation results of handwritten digit recognition.

5.4 Mapping a Second Order Nonlinear System

In the two tasks discussed above, we partitioned the two-dimensional images row-wise and converted spatial patterns into temporal inputs to the reservoir. More native applications of the reservoir system may be to perform temporal data directly, i.e. analyzing time series data and solving dynamic non-linear problems. Figure 5-12 illustrates another experiment where the memristor-based reservoir hardware system is used to solve a second-order dynamic nonlinear task.

Nonlinear dynamical systems are commonly used in electrical, mechanical, control and other engineering fields⁶⁶. Among which, second order nonlinear dynamic systems are widely studied as a model system because of their close relations to electrical systems (i.e. RLC circuits). Figure 5-12 shows the schematic of using an RC system to solve a second order dynamic nonlinear system. For a given input u(k) at timeframe k, the system generates an output y(k) following a nonlinear transfer function that may have a time lag. In our experiment, we choose a 2nd-order

dynamic nonlinear transfer function following a prior study⁶⁷, described as:

$$y(k) = 0.4y(k-1) + 0.4y(k-1)y(k-2) + 0.6u^{3}(k) + 0.1$$
 (5-1)

As can be observed from Equation (5-1), the output y(k) at timeframe k not only depends on the current input u(k), but is also related to the cross term of past two *outputs*, y(k-1) and y(k-2) at timeframes k-1 and k-2, which makes it a 2nd order nonlinear system with a time-lag of two timesteps. In typical applications, the relationship between y(k) and u(k) is implicit and hidden, which makes the problem difficult to solve.



Figure 5-12: Schematic showing the memristor reservoir mapping an unknown nonlinear dynamic system.

The original input signals u() are fed into the original 2nd-order nonlinear system and the output signals y() are generated (upper branch). The same inputs when fed into a memristor reservoir can generate different reservoir states, which are in turn used by the readout function to produce the predicted output p().

The goal is to train the memristor-based RC system to map the hidden nonlinear transfer function, so the correct output y(k) can be obtained from the input u(k) after training, without knowing the original expression between u(k) and y(k).

We note this type of nonlinear problems are well suited for reservoir systems such as the one presented here, since each output y(k) is dependent on the recent past results but not on the far past, matching well with systems having short-term memory effects. We use a 300 timeframe-long random sequence based on uniform random distribution as inputs to train and test the memristor-based RC system for the 2nd order dynamic task implementation, which are shown in Figure 5-13a and b.

$$u(k) = rand[0, 0.5] \tag{5-2}$$

The amplitude of the input signal u(k) is linearly converted into a voltage pulse with amplitude V(k) that is then applied to the memristor reservoir:

$$V(k) = 2 * u(k) + 0.8 \tag{5-3}$$

This linear conversion allows the input voltage pulses to fall in the range of 0.8V-1.8V for memristor stimulation. After collecting the reservoir output, the data is fed into the readout function. Following a similar approach in a prior study⁶⁸, we ignore the first 50 initial data points in the transient period and train the readout function weights w_i (i=1,...90) using the last 250 points in the training sequence using simple linear regression. The same training procedure is also applied for the linear network case used for comparison analysis.

The reservoir consists of 90 physical memristor devices chosen from the memristor crossbar array, and is divided into 10 groups with 9 devices in each group. Input voltage pulse streams with 10 different timeframe widths (1ms, 2ms, 3ms, 4ms, 5ms, 6ms, 8ms, 10ms, 15ms, 20ms) are then respectively applied to the 10 groups through the test board. We found having 9 devices in each group improves the reservoir performance due to inherent device variations that help make the reservoir output more separable, as well as having inputs with different timeframe widths as has already been discussed in the MNIST case. The readout layer in this case is a 90×1 feedforward layer, and is used to convert the reservoir output to a single output y(k). A simple linear regression training algorithm based on batch gradient descent is used to train the readout function.

Suppose the reservoir state is x, which is represented by a vector containing n elements (the conductance values of the n memristors forming the reservoir). The vector representing the reservoir state is applied to the readout network.

The cost function is defined as:

$$J(\mathbf{\theta}) = \frac{1}{2m} \sum_{i=1}^{m} \left(\mathbf{\theta}^{\mathrm{T}} \mathbf{x}^{(i)} - \mathbf{y}^{(i)} \right)^{2}$$
(5-4)

where *m* is the number of samples, $\mathbf{y}^{(i)}$ is the desired output for input $\mathbf{x}^{(i)}$.

To minimize the cost function, the network is trained using the gradient descent defined as

$$\frac{\partial J(\mathbf{\theta})}{\partial \mathbf{\theta}_j} = \frac{1}{m} \sum_{i=1}^m \left(\mathbf{\theta}^{\mathrm{T}} \mathbf{x}^{(i)} - \mathbf{y}^{(i)} \right) \mathbf{x}_j^{(i)}$$
(5 - 5)

Figure 5-13c shows the experimentally-obtained reconstructed (i.e. predicted) outputs from the physical memristor RC system after training (red cycles and dashed line), and the theoretical output (i.e. ground truth) y(k) (blue solid line) from the training sequence, showing the memristor RC system can correctly solve the dynamic nonlinear problem, with a normalized mean squared error (NMSE) of 3.61×10^{-3} . More importantly, to verify the memristor RC system has indeed solved the dynamic transfer function, we tested the system using a new, independently generated random sequence (Figure 5-13b) other than the training sequence. Figure 5-13d shows that the system is still able to successfully predict the expected dynamic output for the random, untrained sequence using the same readout function, with a similar NMSE of 3.13×10^{-3} .



Figure 5-13: Second order nonlinear system results with memristor reservoir a) Uniform random signals u_{train}() are used as the training input. b) Theoretical output y() (blue solid line) vs. experimentally reconstructed output p() from the memristor reservoir computing system (red circles and dashed line), for 100 timeframes from the random training set. c) Another set of uniform random signals u_{test}() are used to test the RC performance. d) Theoretical output y() (blue solid line) vs. experimentally reconstructed output p() from the memristor RC system (red circles and dashed line), for 100 timeframes from the random untrained test set. The readout function was not re-trained in the test

It is worth mentioning that all the preprocessing and training operations used in the 2nd-order nonlinear dynamic task are based on linear transformation. As a result, the nonlinear transformation required by the task has to originate from the intrinsic nonlinear physics of the memristor device.

To highlight the computing capacity provided by the memristor reservoir, we compared the RC system performance against a linear network of the same size. We replaced the memristor reservoir layer with a linear hidden layer, which generates 90 randomly linearly scaled signals of the original input u(k), with scaling factors:

$$x(k) = 2 * rand(0,1) * u(k)$$
 (5-6)

where the x(k) is scaled and from the original input signal u(k), similar to a current value through a linear resistor. In this case, there is no longer any nonlinear transform provided by the reservoir.

We then repeated the signal reconstruction experiments in Figure 5-13c and Figure 5-13d using the linear network with the same training and testing data sets and the same training procedure. The results (Figure 5-14) show that the linear network is not able to solve the dynamic nonlinear problem, and exhibits large errors of 2.23×10^{-1} for the training set and 1.67×10^{-1} for the testing set.



Figure 5-14: Signal reconstruction with a linear system 100 points of the theoretical (blue solid line) and experimental reconstructed outputs (red circle line) of the training data (upper plot) and testing data (lower plot) are shown for the conventional network.

We also calculated the output NMSE for the linear network and the memristor RC system vs. the readout network size (which equals the number of devices n in the reservoir layer since the readout layer is an $n \times 1$ network). Here results from the memristor-based RC system were obtained experimentally using the test board, while results from the linear network were obtained from software. As can be observed from Figure 5-15, the memristor RC system significantly outperforms the linear network having the same size, when solving this dynamic nonlinear task. Additionally, the performance of the memristor RC system is generally improved when using multiple memristor devices in each group, since the inherent device variations increases the reservoir output dimension and thus help improve reservoir state separation.



Figure 5-15: Comparison of the NMSE between the memristor RC system and a linear network. The number of devices in each group in the reservoir layer is increased from 1 to 9 in these tests. The reservoir consists of 10 such groups

5.5 Conclusion

To reduce the training cost needed for temporal data processing, Reservoir Computing is proposed as a variant of recurrent neural network structure. In an RC system only the readout function, i.e. the connections from the reservoir to the output, needs to be trained. In this study, we showed WO_x memristors with short-term memory properties can be used to effectively implement RC systems. We demonstrate experimentally that even a small reservoir consisting of 88 memristor devices can be used to process real-world problems such as handwritten digit recognition with performance comparable to those achieved in much larger networks. A similar-sized network is also used to solve a 2^{nd} -order nonlinear dynamic problem and is able to successfully predict the expected dynamic output without knowing the form of the transfer function.

Chapter 6 Current and Future Works

In the previous chapters, we discussed examples of implementing neuromorphic computing systems with WO_x memristors, from different device behaviors to fully functional integrated circuits. We have successfully demonstrated WO_x memristor crossbar array-based vector-matrix multiplication accelerators for conventional machine learning tasks such as perceptron learning and sparse coding. By using the intrinsic short-term memory dynamics of the device, we can also implement reservoir computing systems that are efficient at processing temporal information.

In this chapter, we discuss a few current and future studies that aim at solving other tasks efficiently with the memristor crossbar structures, namely, Hopfield Networks and self-organizing maps.

6.1 Hopfield Network

A Hopfield Neural Network (HNN) is a form of recurrent artificial neural network popularized by John Hopfield in 1982⁶⁹. The most important property of a Hopfield network is that when updated asynchronously, it guarantees to converge to a stable state in a finite number of steps, which corresponds to an energy local minimum of the network. Since the energy equation is isomorphic to the Hamiltonian of an Ising model, HNNs can be used to solve NP-hard problems⁷⁰.

6.1.1 **Properties and Structure**

Hopfield network is a type of recurrent neural network that does not contain self-connection (or have a self-feedback weight of 0)⁷¹. Typically, in a Hopfield network, a neuron receives the outputs of all other neurons as its input, as shown in Figure 6-1.



Figure 6-1: An illustration of a 4-node Hopfield Neural Network

By simply reorganizing the plot, Figure 6-1 can be converted to a graph shown in Figure 6-2.



The weight between neuron i and j (w_{ij}) is symmetric.

By using a symmetric matrix with a zero diagonal, we can implement the weights of a Hopfield network as a $n \times n$ matrix.

$$W = \begin{pmatrix} 0 & w_{12} & \dots & w_{1n} \\ w_{21} & 0 & \dots & w_{2n} \\ \vdots & \ddots & \vdots \\ w_{n1} & w_{n2} & \dots & 0 \end{pmatrix}$$
(6-1)

The Hopfield network is a dynamical system that can be described as:

$$u_i = \sum_{j}^{n} w_{ij} v_j \tag{6-2a}$$

$$v_{i} = \begin{cases} +1, & if \ u_{i} \ge \theta_{i} \\ -1, & otherwise \end{cases}$$
(6 - 2b)

where is the u_i weighted sum of neuron *i*, v_i is the state of neuron *i*, and θ_i is the threshold of neuron *i*.

By asynchronously update the Hopfield network, the network can eventually converge to a fixed point, which corresponding to the local minima of the following energy function:

$$E = -\frac{1}{2} \sum_{i,j}^{N} w_{ij} v_i v_j + \sum_{i}^{N} \theta_i v_i$$
 (6-3)

This beneficial property of Hopfield network facilitate to solve large optimization problems.

6.1.2 Memristor Implementation

From Equation (6-2a), we can notice that the key operation of a Hopfield network is also vector-matrix multiplication. It is thus naturally suitable to be implemented with a memristor crossbar array, with the weight matrix W programmed into the memristor crossbar. With the high density and analog switching behavior of memristor array, one should be able to implement large scale Hopfield network⁷².



Figure 6-3: Schematic of the Hopfield network implemented by a memristor crossbar array. Image adapted from Reference [72]. Image credit: Dr. Suhas Kumar

In this implementation, the weight of the Hopfield network can be binary or analog depending on the specific problem to be solved. For example, in the case of solving a unweighted Max-cut problem⁷³, the weight matrix *W* is either 0 or -1, which can easily map to low conductance and high conductance of the memrsitor devices in the array. By iteratively calculating the VMMs using parallel read and updating the neuron states, the Hopfield network can converge to a fixed point solution to the NP hard problem.

One advantage of implementing Hopfield network with memristors is that the weight matrix only need to be programmed once, and most of the operations are performing inference, *i.e.* calculating vector-matrix multiplication, which can be done parallelly with very low energy cost. Compared with other approaches such as quantum annealing (e.g. D-wave), the memristor crossbar implementation should be able to achieve better efficiency in energy and area.

The major challenge of this approach is the fact that Hopfield network can easily stuck at local minimums and does not guarantee to find best solution. To solve this issue, an approach of introducing stochastic noise to improve Hopfield network performance will be studied in future works.

6.2 Self-Organizing Map

A Self-organizing Map (SOM) is a data visualization technique developed by Professor Teuvo Kohonen in the early 1980's⁷⁴. It is an unsupervised learning algorithm that transforms high-dimensional data onto lower dimensional subspaces where geometric relationships between points indicate their similarity. The reduction in dimensionality that SOMs provide allows people to visualize and interpret what would otherwise be, for all intents and purposes, indecipherable data.



Figure 6-4: Illustration of a self-organizing map

6.2.1 Training Algorithm

SOMs generate subspaces with unsupervised learning through a competitive learning algorithm. Neuron weights are adjusted based on their proximity to "winning" neurons (i.e. neurons that most closely resemble a sample input). Training over several iterations of input data sets results in similar neurons grouping together and vice versa.

There are two major steps in the SOM training algorithm

1. Given an input sample from the data set, it will select the best matching unit (BMU), which is the so-called winning neuron from all the neurons. The besting matching unit is determined by the Euclidean distance from the neuron and the input

$$dist = \sqrt{\sum_{i=0}^{d} (V_i - W_i)^2}$$
(6-4)

where V is the input sample and W is the neuron to compare. d is the dimension of the data.

2. After finding the winning neuron, it will not only update itself, but also adjust the weights of some nearby neurons within the topological neighborhood. During the training process, the size σ of the neighborhood needs to decrease with time and eventually shrink to 1. Usually the time dependence is an exponential decay:

$$\sigma(t) = \sigma_0 \exp\left(-\frac{t}{\lambda}\right) \tag{6-5}$$

The topological neighborhood is then defined with a Gaussian function as:

$$h(t) = \exp\left(-\frac{dist^2}{2\sigma^2(t)}\right) \tag{6-6}$$

The weights of the neuron are adjusted as:

$$W(t+1) = W(t) + \eta h(t) (V(t) - W(t))$$
(6-7)

6.2.2 Memristor Implementation

Unlike the previously discussed Hopfield network implementation that only perform inference, Self-organizing Map is an online learning algorithm which requires adaptively tuning the network weights, and can thus be more challenging. However, by taking advantages of the intrinsic nonlinear characteristics of the memristor devices, the learning processing can potentially be simplified.

First of all, in SOM, the weight of a neuron usually has multiple dimensions. For example, if the training data are RGB colors, then we can use three devices at the same column as the weight of a neuron, namely:

$$W = [w_R, w_G, w_B]^T (6-8)$$

In this case, each neuron requires three rows to implement. To implement an 8×8 SOM, we need a memristor array of 3×64 , which is a fairly asymmetric size to fit in a square array. By folding the memristor array into multiple rows and use time multiplexing, we can instead use a 12×16 subarray from a 16×16 array.



Figure 6-5: Folding the memristor array to fit in a square array. By storing the weight in a folded matrix and read each three-row batch with time multiplexing, we can transform a 3×64 weight matrix into a 12×16 one.

The key steps in the training algorithm are to find the best matching unit (*i.e.* the winning neuron) and to perform nonlinear weight update at different distances.

Finding the BMU is essentially calculating the minimum of the Euclidean distance, which is very similar to the winner-take-all approach discussed in Chapter 3. By using memristor crossbar structure, we can easily convert the calculation of the Euclidean distance to the comparison of the dot-product value, reducing the computation complexity. To avoid the lack of normalization issue discussed in section 3.3.2, we can use some correction method introduced in the reference⁷⁵ to improve the accuracy in calculating Euclidean distance.

Another challenge is the implementation of the gaussian function to calculate the topological neighborhood, which requires significant pre-processing in the training process. However, since the memristor device exhibits an exponentially nonlinear weight update function vs the applied voltage¹⁸, we can obtain the desired exponentially varying weight changes in Equation (6-7) by simply using a linear decaying programming voltage, with further distance from the winning neuron in the 2-D map corresponding to lower programming voltage. With this approach, the most computational expensive part in training can be simplified by device intrinsic physics.

Further works will focus on the experimental implementation of the SOM on a 12×16 memristor that aims at clustering different RGB colors.

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